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New optimized estimators for the primordial trispectrum

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ABSTRACT

Cosmic microwave background studies of non-Gaussianity involving higher order multispectra can distinguish between early universe theories that predict nearly identical power spectra. However, the recovery of higher order multispectra is difficult from realistic data due to their complex response to inhomogeneous noise and partial sky coverage, which are often difficult to model analytically. A traditional alternative is to use one-point cumulants of various orders, which collapse the information present in a multispectrum to one number. The disadvantage of such a radical compression of the data is a loss of information as to the source of the statistical behaviour. A recent study by Munshi & Heavens has shown how to define the skew spectrum (the power spectra of a certain cubic field, related to the bispectrum) in an optimal way and how to estimate it from realistic data. The skew spectrum retains some of the information from the full configuration dependence of the bispectrum and can contain all the information on non-Gaussianity. In this study, we extend the results of the skew spectrum to the case of two degenerate power spectra related to the trispectrum. We also explore the relationship between these power spectra and cumulant correlators previously used to study non-Gaussianity in projected galaxy surveys or weak-lensing surveys. We construct nearly optimal estimators for quick tests and generalize them to estimators which can handle realistic data with all their complexity in a completely optimal manner. Possible generalizations for arbitrary order are also discussed.

Key words: methods: analytical – methods: numerical – methods: statistical – large-scale structure of Universe.

1 INTRODUCTION

The inflationary paradigm, which solves the flatness, horizon and monopole problem, makes clear predictions about the generation and nature of density perturbations (Starobinsky 1979; Guth 1981; Sato 1981; Albrecht & Steinhardt 1982; Linde 1982). Inflationary models predict the statistical nature of these fluctuations, which are being tested against data from a range of recent cosmological observations, including the recently launched all-sky cosmic microwave background (CMB) survey *Planck*.¹ Various ground-based and space-based observations have already confirmed the generic predictions of inflation, including a flat or nearly flat universe with nearly-scale-invariant adiabatic perturbations at large angular scales. Several planned missions are also targeting the detection of the gravitational wave background through polarization experiments – another generic prediction of inflationary models. The other major prediction of the inflationary scenarios is the nearly Gaussian nature of these perturbations. In the standard slow-roll paradigm, the scalar field responsible for inflation fluctuates with a minimal amount of self-interaction, which ensures that any non-Gaussianity generated during the inflation through self-interaction would be small (Salopek & Bond 1990, 1991; Falk et al. 1993; Gangui et al. 1994; Acquaviva et al. 2003; Maldacena 2003). See Bartolo, Matarrese & Riotto (2006) for a recent review and more detailed discussion. Any detection of non-Gaussianity would therefore be a measure of self-interaction or non-linearities involved, which can come from various alternative scenarios, such as curvaton mechanism, warm inflation, ghost inflation as well as string theory inspired D-acceleration and Dirac Born Infeld models of inflation (Linde & Mukhanov 1997; Gupta et al. 2002; Lyth, Ungarelli & Wands 2003; Alishahiha, Silverstein & Tong 2004; Arkani-Hamed et al. 2004; Chen et al. 2006; Chen, Easther & Lim 2007; Buchbinder, Khoury & Ovrut 2008; Cheung et al. 2008).

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¹ <http://www.rssd.esa.int/index.php?project=Planck>

Early observational work on detection of primordial non-Gaussianity from the *COBE* (Komatsu et al. 2002) and *MAXIMA* (Santos et al. 2003) was followed by much more accurate analysis with the *WMAP*² (Komatsu et al. 2003; Creminelli et al. 2007a; Spergel et al. 2007). Optimized three-point estimators were introduced by Heavens (1998) and have been successively developed (Komatsu, Spergel & Wandelt 2005; Creminelli et al. 2006; Smith & Zaldarriaga 2006; Creminelli, Senatore & Zaldarriaga 2007b; Smith, Zahn & Dore 2007). Indeed, now an estimator for f_{NL} , which saturates the Cramer–Rao bound, has been found, capable of treating partial sky coverage and inhomogeneous noise (Smith, Senatore & Zaldarriaga 2009). The recent claim of detection of non-Gaussianity in *WMAP* data (Yadav & Wandelt 2008) has given a tremendous boost to the study of primordial non-Gaussianity, as it can lift the degeneracy between various early-universe theories, which predict nearly the same primordial power spectrum. Most detection strategies focus on lowest order in non-Gaussianity, that is, the bispectrum or three-point correlation functions (Creminelli 2003; Komatsu et al. 2005; Cabella et al. 2006; Creminelli et al. 2006; Medeiros & Contaldo 2006; Liguori et al. 2007; Smith et al. 2009). This is primarily because of a decrease in signal-to-noise ratio (S/N) as we move up in the hierarchy of correlation functions – the higher order correlation functions are more dominated by noise than their lower order counterparts. Another related complication arises from the necessity to optimize such estimators, and the impact of inhomogeneous noise and partial sky coverage is always difficult to include in such estimates.

The recent study by Munshi & Heavens (2010) suggested the possibility of finding optimized cumulant correlators associated with higher order multispectra in the context of CMB studies. These correlators are well studied in the context of projected surveys, such as projected galaxy surveys, or in the context of weak-lensing studies using simulated maps (Munshi 2000; Munshi & Coles 2000; Munshi & Jain 2000, 2001). Early studies involving cumulant correlators focused mainly on understanding gravity-induced clustering in collisionless media and were widely employed in many studies involving numerical simulations. Cumulant correlators are multipoint correlation functions, collapsed to two points. Although they are two-point correlators, they carry information on the corresponding higher order correlation functions. Due to their *reduced* dimensionality, they do not carry all the information that is encoded in higher order correlation functions, but they carry more than their one-point counterparts, namely the moments of the probability distribution function, which are often used as clustering statistics (Munshi, Melott & Coles 2000; Bernardeau et al. 2002).

One of the reasons to go beyond the lowest order in non-Gaussianity was pointed out by many authors, including, for example, Riquelme & Spergel (2007). At smaller angular scales, the secondary effect may dominate (Spergel et al. 1999a,b; Munshi et al. 1995), in direct contrast to larger angular scales where the anisotropies are generated mainly at the surface of the last scattering. These secondary perturbations are produced by interaction of CMB photons at much lower redshift with the intervening large-scale matter distribution. Such effects will be directly observable with *Planck*. The deflection of CMB photons by the large-scale mass distribution offers the possibility of studying the statistics of density perturbations in an unbiased way and provides clues to growth of structure formation for most part of the cosmic history. Weak lensing of the CMB can provide valuable information for constraining neutrino mass, dark energy equation of state and also has the potential to assist in detection of primordial gravitation waves through CMB polarization information (see e.g. Lewis & Challinor 2006 for a recent review). However, weak-lensing studies using the CMB need to address the contamination produced by other secondaries, such as the thermal Sunyaev–Zel’dovich (tSZ) effects and kinetic Sunyaev–Zel’dovich (kSZ) effect as well as by point sources, although it is believed that these contaminations are not so important in case of polarization studies. It was pointed out in Riquelme & Spergel (2007) that a real-space statistic, such as $\langle \delta T^3(\hat{\Omega}) \delta T(\hat{\Omega}') \rangle_c$ (which is a cumulant correlator of the order of 4) can be used to separate the kSZ effect or Ostriker–Vishniac effect from the lensing effect as the lensing contribution cancels out at the lowest order. It was shown that, in addition to quantifying and controlling the kSZ contamination of lensing statistics, such statistics could as well play a very important role in providing new insight into the history of reionization. In a completely different context, it was shown that this estimator has also been used for testing models of primordial non-Gaussianity using redshifted 21-cm observations (Cooray 2006; Cooray, Li & Melchiorri 2008). While cumulant correlators at third order $\langle \delta T^2(\hat{\Omega}) \delta T(\hat{\Omega}') \rangle_c$ can provide information regarding the non-Gaussianity parameter f_{NL} , fourth-order statistics, such as $\langle \delta T^2(\hat{\Omega}) \delta T^2(\hat{\Omega}') \rangle_c$, can go beyond the lowest-order non-Gaussianity by putting constraints on the next-order parameter g_{NL} (to be introduced in later sections), albeit at lower S/N. However, with ongoing CMB missions, such as *Planck*, the situation will improve and developing optimal methods for such higher order cumulant correlators is the first step in this direction. There are now several studies which provide independent estimates of f_{NL} ; however, we still lack such constraints for g_{NL} . This clearly is related to the fact that in typical models, g_{NL} is expected to be small, $g_{NL} \leq r/50$, where r is the scalar-to-tensor ratio (Seery, Lidsay & Sloth 2007). We also note that various studies have pointed out the link between the non-Gaussianity analysis and the estimators, which test the anisotropy of the primordial universe. We plan to address these issues in a related publication. Several inflationary models provide direct consistency relations between f_{NL} and g_{NL} , for example, $g_{NL} = (6f_{NL}/5)^2$ (in some publications, it is also denoted by f_2 or τ_{NL} , for example, Hu & Okamoto 2002; Cooray 2006; Seery et al. 2007). Testing of these consistency relations can give valuable clues to the mechanism behind the generation of initial perturbations. However, a difficulty for methods designed to detect non-Gaussianity in the CMB is that other processes can contribute, such as gravitational lensing, unsubtracted point sources and imperfect subtraction of galactic foreground emission discussed by, for example, Goldberg & Spergel (1999), Cooray & Hu (2000), Verde & Spergel (2002), Castro (2004) and Babich & Pierpaoli (2008).

While the main motivation in this work is to study the primordial trispectrum, we note that mode–mode coupling resulting from weak lensing of the CMB produces a trispectrum, which has been studied using power spectra associated with $\langle \delta T(\hat{\Omega})^2 \delta T(\hat{\Omega}')^2 \rangle_c$. Lensing studies involving the CMB can achieve higher S/N at the level of the bispectrum, if we use external data sets to act as tracers of large-scale structure.

² <http://map.gsfc.nasa.gov/>

However, the lowest order at which the internal detection of CMB lensing is possible is the trispectrum. There have been some attempts to detect non-Gaussianity at the level of the trispectrum using, for example, the *COBE* 4-yr data release (Kunz et al. 2001), BOOMERanG data (Troia et al. 2003) and more recently using *WMAP* 3-yr data (Spergel et al. 2007).

The layout of this paper is as follows. In Section 2, we introduce the concept of higher order cumulant correlators and how they are linked to corresponding correlation functions in real space. In Section 3, we discuss harmonic transforms of cumulant correlators and their relations to the corresponding multispectra. We also discuss estimators based on pseudo- C_l (PCL) estimators used for power spectrum estimation and generalize them to two-point cumulant correlators at higher order in this section. In Section 4, we briefly discuss the ‘*local*’ models for initial perturbations and the resulting trispectrum. These models are then used in Section 4 to optimize the power spectra associated with the multispectra. This approach is nearly optimal, describing the mode–mode coupling using the ‘*fraction of sky*’ approach discussed in other studies. In Section 5, we present an estimator, which is nearly optimal and can take into account partial sky coverage as well as realistic inhomogeneous noise resulting from the scanning strategy. This estimator can work directly with any specific theoretical model for primordial trispectra, based on concepts of matched filtering, and generalizes the results obtained previously by Munshi & Heavens (2010). We present results for one-point estimators and also generalize them to two corresponding power spectra. Section 6 is devoted to adding relevant linear correction terms to these estimators in the absence of spherical symmetry. Next, in Section 7, we introduce inverse covariance weighting and design a trispectrum estimator, which is optimal for arbitrary scanning strategy. The estimator used in this section will also be useful in estimating secondary non-Gaussianity. For homogeneous noise and all-sky coverage, the estimators are identical. Finally, Section 8 is devoted to concluding discussions and future prospects.

2 CORRELATION FUNCTIONS AND THE CUMULANT CORRELATORS

The temperature fluctuations of the CMB are typically assumed to be a realization of statistically isotropic Gaussian random field. For Gaussian perturbations, all the information needed to provide a complete statistical description is contained in the power spectrum of the distribution; for a non-Gaussian distribution, higher order correlation functions are also needed. With the assumption of *weak* non-Gaussianity, only the first few correlation functions are needed to describe the departure from Gaussianity. We will denote the n -point correlation function by $\xi_N(\hat{\Omega}_1, \dots, \hat{\Omega}_n)$. The n -point correlation functions are decomposed into parts, which are purely Gaussian in nature and those which signify departures from Gaussianity. These are also known as *connected* and *disconnected* terms because of their representation by respective diagrams (see Bernardeau et al. 2002 for more details). At the level of the four-point correlation function, the corresponding connected part, denoted by the subscript $\langle \dots \rangle_c$, μ_4 can be defined as

$$\mu_4(\hat{\Omega}_1, \dots, \hat{\Omega}_4) = \langle \delta T(\hat{\Omega}_1) \dots \delta T(\hat{\Omega}_4) \rangle_c. \quad (1)$$

The connected component of the four-point function will be exactly zero for a purely Gaussian temperature field. The Gaussian contribution, on the other hand, can be written as a product of two two-point correlation functions. So, the total four-point correlation function can be written as the sum of the connected and the disconnected parts:

$$\xi_4(\hat{\Omega}_1 \dots \hat{\Omega}_4) = \xi_2(\hat{\Omega}_1, \hat{\Omega}_2)\xi_2(\hat{\Omega}_3, \hat{\Omega}_4) + \xi_2(\hat{\Omega}_1, \hat{\Omega}_3)\xi_2(\hat{\Omega}_2, \hat{\Omega}_4) + \xi_2(\hat{\Omega}_1, \hat{\Omega}_4)\xi_2(\hat{\Omega}_2, \hat{\Omega}_3) + \mu_4(\hat{\Omega}_1 \dots \hat{\Omega}_4). \quad (2)$$

As we will see, the Gaussian part will add to the scatter associated with any estimator for the four-point correlation function. At lower level $\xi_2(\hat{\Omega}_1, \hat{\Omega}_2) = \mu_2(\hat{\Omega}_1, \hat{\Omega}_2)$ and $\xi_3(\hat{\Omega}_1 \dots \hat{\Omega}_3) = \mu_3(\hat{\Omega}_1 \dots \hat{\Omega}_3)$ and hence there are no disconnected parts. The number of degrees of freedom associated with higher order correlations increases exponentially with its order. This is mainly due to the increased number of configurations possible for which one can measure a higher order correlation function. The cumulant correlators are defined by identifying all available vertices or points to just two points. There are two such cumulant correlators, which can be constructed at the four-point level:

$$\xi_{31} \equiv \langle \delta^3 T(\hat{\Omega}_1) \delta T(\hat{\Omega}_2) \rangle_c; \quad \xi_{22} \equiv \langle \delta^2 T(\hat{\Omega}_1) \delta T^2(\hat{\Omega}_2) \rangle_c. \quad (3)$$

These two degenerate sets of cumulant correlators carry information at the level of four-point, but they are essentially two-point correlation functions and can be studied in the harmonic domain by their associated power spectra. The first, ξ_{31} , was studied in the context of 21-cm surveys by Cooray (2006) and Cooray et al. (2008), and the second, ξ_{22} , was shown to have the power to separate the lensing contribution from the kSZ effect (Riquelme & Spergel 2007). These are natural generalizations of their third-order counterpart recently studied by Munshi & Heavens (2010) who introduced their optimized form for direct use on realistic data. These were later used by Smidt et al. (2009) to estimate f_{NL} and by Calabrese et al. (2009) to study lensing-secondary correlations from *WMAP5* data.

Although there are various advantages of working in real space, it is often easier to work in the harmonic domain. The main motivation to work in the harmonic domain is linked to the fact that inflationary models predict a well-defined peak structure for the power spectrum. These structures are well-known diagnostics for constraining cosmology at various levels. This is true for higher order multispectra as they also involve the effect of the transfer functions. Note that the noise in CMB experiments is typically assumed to be Gaussian and will therefore contribute only to the disconnected terms.

3 FOURIER TRANSFORMS OF CUMULANT CORRELATORS AND THEIR OPTIMUM ESTIMATORS

The real-space correlation functions are clearly very important tools, which can be used in surveys with patchy sky coverage. However, recent CMB surveys scan the sky with near all-sky coverage. This makes a harmonic-space description more appropriate as various symmetries can be included in a more straightforward way. For Gaussian random fields with all-sky coverage, the estimates of various statistics are, loosely

speaking, uncorrelated. Even for a non-Gaussian field, they are reasonably uncorrelated at different angular scales or at different l as long as the non-Gaussianity is weak. We begin by introducing the harmonic transform of the observed temperature map $\delta T(\hat{\Omega})$ ($\hat{\Omega} = (\theta, \phi)$) for all-sky coverage:

$$a_{lm} \equiv \int d\hat{\Omega} \frac{\Delta T(\hat{\Omega})}{T} Y_{lm}^*(\hat{\Omega}) \equiv \int d\hat{\Omega} \delta T(\hat{\Omega}) Y_{lm}^*(\hat{\Omega}). \quad (4)$$

Realistically, however, we will only be observing the part of the sky which is not masked by Galactic foregrounds. The window function $w(\Omega)$, which we will take as a completely general window, can be used to define what is known as the pseudo-harmonics, which we designate as \tilde{a}_{lm} :

$$\tilde{a}_{lm} \equiv \int d\hat{\Omega} w(\hat{\Omega}) \delta T(\hat{\Omega}) Y_{lm}^*(\hat{\Omega}). \quad (5)$$

We follow this description for the remainder of this paper. Any statistic X obtained from the masked sky will be denoted by \tilde{X} and the estimated all-sky version will be denoted by \hat{X} . The ensemble averages of the unbiased all-sky estimators, which coincide with the theoretical models, will be denoted only by the corresponding latin symbol X .

3.1 Two-point estimators for the trispectrum $C_l^{(3,1)}$, $C_l^{(2,2)}$

At the level of four-point cumulant correlators, we have two different estimators, which can independently be used to study the trispectrum. The estimators that we discuss here are direct harmonic transforms of these two-point correlators. We introduced the cumulant correlators in equation (3). The two estimators we define in this section are related to $\langle \delta T^2(\hat{\Omega}) \delta^2 T(\hat{\Omega}') \rangle$ and $\langle \delta T^3(\hat{\Omega}) \delta T(\hat{\Omega}') \rangle$ through harmonic transforms. For the cubic function $\delta T^3(\hat{\Omega})$, we denote the harmonic transform by $a_{lm}^{(3)}$ and similarly $a_{lm}^{(2)}$ denotes the harmonic transform of the quadratic form $\delta T^2(\hat{\Omega})$. We obtain the following relations for all-sky coverage and for the pseudo-harmonics $\tilde{a}_{lm}^{(2)}$ with a mask³:

$$a_{lm}^{(2)} = \sum_{l_1 m_1} \sum_{l_2 m_2} a_{l_1 m_1} a_{l_2 m_2} \int d\hat{\Omega} Y_{l_1 m_1}(\hat{\Omega}) Y_{l_2 m_2}(\hat{\Omega}) Y_{lm}^*(\hat{\Omega}) \quad (6)$$

and

$$\tilde{a}_{lm}^{(2)} = \sum_{l_1 m_1} \dots \sum_{l_3 m_3} a_{l_1 m_1} a_{l_2 m_2} w_{l_3 m_3} \int d\hat{\Omega} Y_{l_1 m_1}(\hat{\Omega}) Y_{l_2 m_2}(\hat{\Omega}) Y_{l_3 m_3}(\hat{\Omega}) Y_{lm}^*(\hat{\Omega}) = \sum_{(l' m')} K_{lm l' m'} a_{l' m'}^{(2)}, \quad (7)$$

respectively. The corresponding results for $a_{lm}^{(3)}$ and $\tilde{a}_{lm}^{(3)}$ are as follows:

$$a_{lm}^{(3)} = \sum_{l_1 m_1} \dots \sum_{l_3 m_3} a_{l_1 m_1} a_{l_2 m_2} a_{l_3 m_3} \int d\hat{\Omega} Y_{l_1 m_1}(\hat{\Omega}) Y_{l_2 m_2}(\hat{\Omega}) Y_{l_3 m_3}(\hat{\Omega}) Y_{lm}^*(\hat{\Omega}) \quad (8)$$

and

$$\tilde{a}_{lm}^{(3)} = \sum_{l_1 m_1} \dots \sum_{l_4 m_4} a_{l_1 m_1} a_{l_2 m_2} a_{l_3 m_3} w_{l_4 m_4} \int d\hat{\Omega} Y_{l_1 m_1}(\hat{\Omega}) Y_{l_2 m_2}(\hat{\Omega}) Y_{l_3 m_3}(\hat{\Omega}) Y_{l_4 m_4}(\hat{\Omega}) Y_{lm}^*(\hat{\Omega}) = \sum_{(l' m')} K_{lm l' m'} a_{l' m'}^{(3)}. \quad (9)$$

The coupling matrix $K_{lm l' m'}$ encodes information about the mode coupling, which is introduced because of the masking of the sky (Hivon et al. 2002):

$$K_{l_1 m_1 l_2 m_2} [w] = \int w(\hat{\Omega}) Y_{l_1 m_1}(\hat{\Omega}) Y_{l_2 m_2}(\hat{\Omega}) d\hat{\Omega} = \sum_{l_3 m_3} \tilde{w}_{l_3 m_3} \left[\frac{(2l_1 + 1)(2l_2 + 1)(2l_3 + 1)}{4\pi} \right]^{1/2} \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix}. \quad (10)$$

The matrices here denote the Wigner $3j$ -symbols (Edmonds 1968). Using the harmonic transforms, we define the following power spectra, which can directly probe the trispectra:

$$C_l^{(2,2)} = \frac{1}{2l+1} \sum_m a_{lm}^{(2)*} a_{lm}^{(2)}; \quad \tilde{C}_l^{(2,2)} = \frac{1}{2l+1} \sum_m \tilde{a}_{lm}^{(2)*} \tilde{a}_{lm}^{(2)}. \quad (11)$$

From the consideration of isotropy and homogeneity, we can write the following relations:

$$\langle a_{lm}^{(2)} a_{lm}^{(2)*} \rangle_c = C_l^{(2,2)} \delta_{ll'} \delta_{mm'}; \quad \langle a_{lm}^{(3)} a_{lm}^{(3)*} \rangle_c = C_l^{(3,1)} \delta_{ll'} \delta_{mm'}. \quad (12)$$

The pseudo-power spectrum, which is recovered from the masked harmonics, is defined in an analogous way. Finally, the resulting power spectra $C_l^{(2,2)}$ can be expressed in terms of the trispectrum $T_{l_3 l_4}^{l_1 l_2}(l)$ by the following expression:

$$C_l^{(2,2)} = \sum_{l_1 l_2 l_3 l_4} T_{l_3 l_4}^{l_1 l_2}(l) \sqrt{\frac{(2l_1 + 1)(2l_2 + 1)}{4\pi(2l + 1)}} \sqrt{\frac{(2l_3 + 1)(2l_4 + 1)}{4\pi(2l + 1)}} \begin{pmatrix} l_1 & l_2 & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & l \\ 0 & 0 & 0 \end{pmatrix}. \quad (13)$$

³ In this paper, we will consider analysis of Temperature data. Joint analysis of Temperature and Polarization data is presented in Munshi et al. (2010).

The trispectrum, which is introduced here, is a four-point correlation function in harmonic space. The definition here ensures that it is invariant under various transformations (see Hu 2000 and Hu & Okamoto 2002 for detailed discussion):

$$\langle a_{l_1 m_1} a_{l_2 m_2} a_{l_3 m_3} a_{l_4 m_4} \rangle_c = \sum_{LM} (-1)^M T_{l_3 l_4}^{l_1 l_2}(L) \begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & M \end{pmatrix} \begin{pmatrix} l_3 & l_4 & L \\ m_3 & m_4 & -M \end{pmatrix}. \quad (14)$$

Partial sky coverage can be dealt with in an exactly similar manner. By using the harmonic transforms of the masked sky and expressing the masked harmonics in terms of all-sky harmonics, we can relate the PCL versions of these power spectra $\tilde{C}_l^{(2,2)}$ in terms of its all-sky components $C_l^{(2,2)}$. This involves the harmonic transform of the mask W_{lm} and its associated power spectrum W_l . The coupling matrix for $M_{ll'}$ is the same as that used for inverting the PCL power spectrum to recover the unbiased power spectrum:

$$\begin{aligned} \tilde{C}_l^{(2,2)} &= \sum_{l'l''} (2l' + 1) \begin{pmatrix} l & l' & l'' \\ 0 & 0 & 0 \end{pmatrix}^2 \frac{(2l'' + 1)}{4\pi} |w_{l''}^2| \\ &\times \sum_{l_1 l_2 l_3 L} T_{l_3 l_4}^{l_1 l_2}(L) \sqrt{\frac{(2l_1 + 1)(2l_2 + 1)}{4\pi(2l' + 1)}} \sqrt{\frac{(2l_3 + 1)(2l_4 + 1)}{4\pi(2l' + 1)}} \begin{pmatrix} l_1 & l_2 & l' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & l'' \\ 0 & 0 & 0 \end{pmatrix} = \sum_{l'} M_{ll'} C_{l'}^{(2,2)}, \end{aligned} \quad (15)$$

where

$$M_{ll'} = (2l' + 1) \sum_{l''} \begin{pmatrix} l & l' & l'' \\ 0 & 0 & 0 \end{pmatrix}^2 \frac{(2l'' + 1)}{4\pi} |w_{l''}^2|. \quad (16)$$

In the literature, the power spectrum $c_l^{(2,2)}$ is also referred to as the *second spectrum*. The other degenerate cumulant correlator of the same order that contains information about the trispectrum can be written as

$$C_l^{(3,1)} = \frac{1}{2l + 1} \sum_m \text{Real} \left\{ a_{lm}^{(3)*} a_{lm}^{(1)} \right\}; \quad \tilde{C}_l^{(3,1)} = \frac{1}{2l + 1} \sum_m \text{Real} \left\{ \tilde{a}_{lm}^{(3)*} \tilde{a}_{lm}^{(1)} \right\}. \quad (17)$$

The resulting power spectrum, which probes the various components of the trispectrum with different weights, can be expressed as follows:

$$C_l^{(3,1)} = \sum_{l_1 l_2 l_3 L} T_{l_3 l}^{l_1 l_2}(L) \sqrt{\frac{(2l_1 + 1)(2l_2 + 1)}{4\pi(2L + 1)}} \sqrt{\frac{(2L + 1)(2l_3 + 1)}{4\pi(2l + 1)}} \begin{pmatrix} l_1 & l_2 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & l_3 & l \\ 0 & 0 & 0 \end{pmatrix}. \quad (18)$$

With partial sky coverage, we can proceed as before to connect the PCL version of the estimator $\tilde{C}_l^{(3,1)}$ to its all-sky analogue. The resulting estimators combine the values of various components of the trispectrum with different weighting. The associated power spectrum will therefore have a different dependence on parameters describing the primordial trispectrum:

$$\begin{aligned} C_l^{(3,1)} &= \sum_{l'l''} (2l' + 1) \begin{pmatrix} l & l' & l'' \\ 0 & 0 & 0 \end{pmatrix}^2 \frac{(2l'' + 1)}{4\pi} |w_{l''}^2| \\ &\times \sum_{l_1 l_2 l_3 L} T_{l_3 l}^{l_1 l_2}(L) \sqrt{\frac{(2l_1 + 1)(2l_2 + 1)}{4\pi(2L + 1)}} \sqrt{\frac{(2L + 1)(2l_3 + 1)}{4\pi(2l' + 1)}} \begin{pmatrix} l_1 & l_2 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & l_3 & l' \\ 0 & 0 & 0 \end{pmatrix} = \sum_{l'} M_{ll'} C_{l'}^{(3,1)}. \end{aligned} \quad (19)$$

The links to real-space cumulant correlators are the same as their third-order counterpart:

$$\langle \delta^2 T(\hat{\Omega}) \delta^2 T(\hat{\Omega}') \rangle_c = \frac{1}{4\pi} \sum_l (2l + 1) P_l(\cos(\hat{\Omega} \cdot \hat{\Omega}')) C_l^{(2,2)}; \quad \langle \delta^3 T(\hat{\Omega}) \delta T(\hat{\Omega}') \rangle_c = \frac{1}{4\pi} \sum_l (2l + 1) P_l(\cos(\hat{\Omega} \cdot \hat{\Omega}')) C_l^{(3,1)}. \quad (20)$$

Hence, we can conclude that it is possible to generalize these results to an arbitrary mask with arbitrary weighting functions. The deconvolved set of estimators at order p, q can be written as follows:

$$\hat{C}_l^{p,q} = M_{ll'}^{-1} \tilde{C}_{l'}^{p,q}. \quad (21)$$

This is one of the important results of this paper. The mask used for various orders p, q is the same, but with the increasing order the number of degenerate power spectra that can be constructed from a multispectrum increases drastically. As we have seen at the level of bispectrum, we can keep one of the triangle sides fixed and sum over all contributions from all possible configurations of the triangle. Similarly, for the trispectrum, we can keep one of the sides of the rectangle fixed, or one of the diagonals fixed, and sum over all possible configurations. The possibilities increase as we move to higher order in multispectra. Another related complication would be from the number of disconnected terms, which need to be subtracted as they simply correspond to Gaussian contributions. At the four-point level, we need to subtract the disconnected pieces from the dominant Gaussian component of temperature fluctuations including the noise (Hu 2000; Hu & Okamoto 2002):

$$G_{l_3 l_4}^{l_1 l_2}(L) = (-1)^{l_1 + l_3} \sqrt{(2l_1 + 1)(2l_3 + 1)} C_{l_1} C_{l_3} \delta_{L0} \delta_{l_1 l_2} \delta_{l_2 l_3} + (2L + 1) C_{l_1} C_{l_2} \left[(-1)^{l_2 + l_3 + L} \delta_{l_1 l_3} \delta_{l_2 l_4} + \delta_{l_1 l_4} \delta_{l_2 l_3} \right], \quad (22)$$

where C_l is the power spectrum including noise.

For the all-sky case and if we restrict only to modes with ordering $l_1 \leq l_2 \leq l_3 \leq l_4$, the non-zero component corresponds to terms with $L = 0$ or $l_1 = l_2 = l_3 = l_4$. However, for arbitrary sky coverage, which results in mode-mode coupling, no such general comments can be made. Estimators developed here in their all-sky form are known in the literature and the results here show how to generalize them for partial sky coverage. However, the main interest in data compression lies in using optimal weights for the compression, which is model-dependent as the weights depend on the specific model being probed (see Table 1 for notations).

Table 1. Various multispectra and associated power spectra are tabulated along with their cosmological use.

Order	Cumulant and correlator	Power spectra	Use
2 = (1 + 1)	$\langle \delta^2 T(\hat{\Omega}) \rangle, \langle \delta T(\hat{\Omega}) \delta T(\hat{\Omega}') \rangle$	C_l	Constraints on cosmology ($\Omega, H_0 \dots$)
3 = (2 + 1)	$\langle \delta^3 T(\hat{\Omega}) \rangle, \langle \delta^2 T(\hat{\Omega}) \delta T(\hat{\Omega}') \rangle$	$S^{(3)}, S_l^{(2,1)}$	Inflationary models f_{NL} , secondaries x lensing b_l
4 = (3 + 1), (2 + 2)	$\langle \delta^4 T(\hat{\Omega}) \rangle, \langle \delta^3 T(\hat{\Omega}) \delta(\hat{\Omega}') \rangle, \langle \delta^2 T(\hat{\Omega}) \delta^2 T(\hat{\Omega}') \rangle$	$K^{(4)}, K_l^{(2,2)}, K_l^{(3,1)}$	f_{NL}, g_{NL} , kSZ lensing separate internal lensing det.

If we introduce the Gaussian contributions to $C_l^{(3,1)}$ as $G_l^{(3,1)}$ and to $C_l^{(2,2)}$ as $G_l^{(2,2)}$, then in the presence of partial sky coverage, we can write

$$\tilde{G}_l^{(3,1)} = \sum_{l'} M_{ll'} G_{l'}^{(3,1)}; \quad \tilde{G}_l^{(2,2)} = \sum_{l'} M_{ll'} G_{l'}^{(2,2)}. \quad (23)$$

For all-sky coverage, one can obtain the corresponding results by replacing $T_{l_3 l_4}(L)$ by $G_{l_3 l_4}^{l_1 l_2}(L)$ in respective equations:

$$G_l^{(3,1)} = \sum_{l_1 l_2 l_3 L} G_{l_3 l}^{l_1 l_2}(L) \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2L+1)}} \sqrt{\frac{(2L+1)(2l_3+1)}{4\pi(2l+1)}} \begin{pmatrix} l_1 & l_2 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & l_3 & l \\ 0 & 0 & 0 \end{pmatrix}; \quad (24)$$

$$G_l^{(2,2)} = \sum_{l_1 l_2 l_3 l_4} G_{l_3 l_4}^{l_1 l_2}(l) \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l+1)}} \sqrt{\frac{(2l_3+1)(2l_4+1)}{4\pi(2l+1)}} \begin{pmatrix} l_1 & l_2 & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & l \\ 0 & 0 & 0 \end{pmatrix}. \quad (25)$$

To subtract the disconnected Gaussian part, we use simulations. These are constructed from the same power spectrum that describes the non-Gaussian maps. Noise realizations, which describe the actual map, are also introduced in the Gaussian maps and exactly the same mask is used. This will ensure that the estimator remains unbiased. If we denote the final estimators after the subtraction of Gaussian disconnected parts by $\hat{D}_l^{(3,1)}$ and $\hat{D}_l^{(2,2)}$, we can write for all-sky coverage

$$\hat{D}_l^{(2,2)} \equiv \hat{C}_l^{(2,2)} - \hat{G}_l^{(2,2)}; \quad \hat{D}_l^{(3,1)} \equiv \hat{C}_l^{(3,1)} - \hat{G}_l^{(3,1)}. \quad (26)$$

In the presence of a mask, deconvolved estimators are related to the masked estimators by the mixing matrix $M_{ll'}$:

$$\hat{D}_l^{(2,2)} = \sum_{l'} M_{ll'}^{-1} (\tilde{C}_{l'}^{(2,2)} - \tilde{G}_{l'}^{(2,2)}); \quad \hat{D}_l^{(3,1)} = \sum_{l'} M_{ll'}^{-1} (\tilde{C}_{l'}^{(3,1)} - \tilde{G}_{l'}^{(3,1)}). \quad (27)$$

Practical implementation of these estimators can provide a quick sanity check of a pipeline design for non-Gaussian estimators (Cooray 2001; Chen & Szapudi 2006). While it is useful to keep in mind that these estimators are suboptimal, they are nevertheless *unbiased* and, depending on various choices of f_{NL} and g_{NL} , they can provide an analytical basis for computation of the scatter and cross-correlation among various estimators associated with different levels of the correlation hierarchy.

The dependence of $\hat{D}_l^{(2,2)}$ and $\hat{D}_l^{(3,1)}$ on f_{NL} and g_{NL} is different and hence can be used to provide independent constraints on both these parameters without using third-order estimators and might be useful for providing cross-checks.

3.2 One-point unoptimized estimators for the trispectrum μ_4

The one-point cumulants at third order can be written in terms of the bispectra as

$$\mu_3 = \langle \delta T^3(\hat{\Omega}) \rangle = \frac{1}{4\pi} \int \delta T^3(\hat{\Omega}) d\hat{\Omega} = \frac{1}{4\pi} \sum_{l_1 l_2 l_3} h_{l_1 l_2 l_3} B_{l_1 l_2 l_3}. \quad (28)$$

The symbol $h_{l_1 l_2 l_3}$ is defined in equation (41). Similarly, the one-point cumulant at fourth order can be written in terms of the trispectra as

$$\mu_4 = \langle \delta T^4(\hat{\Omega}) \rangle_c = \frac{1}{4\pi} \int \delta T^4(\hat{\Omega}) d\hat{\Omega} = \frac{1}{4\pi} \sum_L \sum_{l_1 l_2 l_3 l_4} h_{l_1 l_2 L} h_{l_3 l_4 L} T_{l_1 l_2}^{l_3 l_4}(L). \quad (29)$$

We can also define the S_N parameters generally used in the literature as

$$S_3 = \mu_3; \quad S_4 = \mu_4 - 3\mu_2^2. \quad (30)$$

Throughout this discussion, we have absorbed the experimental beam $b_l = \exp\{-l(l+1)/2\sigma_b^2\}$ in the harmonics a_{lm} unless it is displayed explicitly. Here $\sigma_b = \text{FWHM}/\sqrt{8 \ln 2}$ for a Gaussian beam (FWHM stands for full width at half-maximum). Alternatively, it is also possible to define by respective powers of μ_2 to make these one-point estimators less sensitive to the normalization of the power spectra. In that case, we will have $S_3 = \mu_3/\mu_2^2$. These moments at fourth order are generalizations of the third-order moments, used as a basis for the construction of estimators for f_{NL} by introducing the optimal weights $A(r, \hat{\Omega})$ and $B(r, \hat{\Omega})$.

4 MODELS FOR PRIMORDIAL NON-GAUSSIANITY AND CONSTRUCTION OF OPTIMAL WEIGHTS

The optimization techniques that we introduce in the next section follow the discussion in Munshi & Heavens (2010). The optimization procedure depends on construction of three-dimensional fields from the harmonic components of the temperature fields a_{lm} with suitable

weighting with respective functions, which describes primordial non-Gaussianity (Yadav, Komatsu & Wandelt 2007). These weights make the estimators to act about optimum and the matched filtering technique adopted ensures that the response to the observed non-Gaussianity is maximum when it matches with primordial non-Gaussianity corresponding to the weights.

In the linear regime, the curvature perturbations, which generate the fluctuations in the CMB sky, are written as

$$a_{lm} = 4\pi(-i)^l \int \frac{d^3k}{(2\pi)^3} \Phi(\mathbf{k}) \Delta_l^T(k) Y_{lm}(\hat{\mathbf{k}}). \quad (31)$$

We will need the following functions to construct the harmonic-space trispectra as well as to generate weights for construction of optimal estimators (for a more complete description of predicting trispectra from a given inflationary prediction, see Hu 2000; Hu & Okamoto 2002):

$$\alpha_l(r) = \frac{2}{\pi} \int_0^\infty k^2 dk \Delta_l(k) j_l(kr); \quad \beta_l(r) = \frac{2}{\pi} \int_0^\infty k^2 dk P_\phi(k) \Delta_l(k) j_l(kr); \quad \mu_l(r) = \frac{2}{\pi} \int_0^\infty k^2 dk \Delta_l(k) j_l(kr). \quad (32)$$

In the limit of low multipoles where the perturbations are mainly dominated by Sachs–Wolfe effect, the transfer functions $\Delta_l(k)$ take a rather simple form $\Delta_l(k) = 1/3j_l(kr_*)$, where $r_* = (\eta_0 - \eta_{\text{dec}})$ denotes the time elapsed between cosmic recombination and the present epoch. In general, the transfer function needs to be computed numerically. The *local* model for the primordial bispectrum and trispectrum can be constructed by going beyond linear theory in the expansion of $\Phi(x)$. The additional parameters, f_{NL} and g_{NL} , are introduced, which need to be estimated from observation. As discussed in the introduction, g_{NL} can be linked to r , the scalar-to-tensor ratio in a specific inflationary model, and hence expected to be small:

$$\Phi(\mathbf{x}) = \Phi_L(\mathbf{x}) + f_{NL} (\Phi_L^2(\mathbf{x}) - \langle \Phi_L^2(\mathbf{x}) \rangle) + g_{NL} \Phi_L^3(\mathbf{x}) + h_{NL} (\Phi_L^4(\mathbf{x}) - 3 \langle \Phi_L^2(\mathbf{x}) \rangle^2) + \dots \quad (33)$$

We will only consider the local model of primordial non-Gaussianity in this paper and adiabatic initial perturbations. More complicated cases of primordial non-Gaussianity will be dealt with elsewhere. In terms of an inflationary potential, $V(\phi)$, associated with a scalar potential ϕ and its derivatives, one can express parameter constants f_{NL} and g_{BL} as derived in Hu (2000).

There are two contributions to primordial non-Gaussianity. The first part is parametrized by f_{NL} and the second contribution is proportional to a new parameter, which appears at fourth order, denoted by g_{NL} . From theoretical considerations, in generic models of inflation, one would expect $g_{NL} \leq r/50$ with r being the scalar-to-tensor ratio (Seery et al. 2007).

Following Hu (2000), we can expand the above expression in Fourier space to write

$$\Phi_2(k) = \int \frac{d^3\mathbf{k}_1}{(2\pi)^3} \Phi_L(\mathbf{k} + \mathbf{k}_1) \Phi_L^*(\mathbf{k}_1) - (2\pi)^3 \delta_D(\mathbf{k}) \int \frac{d^3\mathbf{k}_1}{(2\pi)^3} P_\Phi(\mathbf{k}_1); \quad (34)$$

$$\Phi_3(k) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \Phi_L(\mathbf{k}_1) \Phi_L(\mathbf{k}_2) \Phi_L^*(\mathbf{k}_1). \quad (35)$$

The resulting trispectra associated with these perturbations can be expressed as

$$T_\Phi(k_1, k_2, k_3, k_4) \equiv \langle \delta(\mathbf{k}_1) \delta(\mathbf{k}_2) \delta(\mathbf{k}_3) \delta(\mathbf{k}_4) \rangle_c = \int \frac{d^3\mathbf{K}}{(2\pi)^3} \delta_D(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{K}) \delta_D(\mathbf{k}_3 + \mathbf{k}_4 + \mathbf{K}) \mathcal{T}_\Phi(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4, \mathbf{K}). \quad (36)$$

where $\mathcal{T}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4, \mathbf{K})$ can be decomposed into the following two different constituents:

$$\mathcal{T}_\Phi^{(2)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4, \mathbf{K}) = 4f_{NL}^2 P_\Phi(\mathbf{K}) P_\Phi(\mathbf{k}_1) P_\Phi(\mathbf{k}_3); \quad (37)$$

$$\mathcal{T}_\Phi^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4, \mathbf{K}) = g_{NL} \{ P_\Phi(\mathbf{K}) P_\Phi(\mathbf{k}_1) P_\Phi(\mathbf{k}_3) + P_\Phi(\mathbf{K}) P_\Phi(\mathbf{k}_1) P_\Phi(\mathbf{k}_3) \}. \quad (38)$$

The *reduced* CMB trispectrum can now be written as

$$\tau_{l_1 l_2 l_3 l_4}^{l_1 l_2}(L) = 4f_{NL}^2 h_{l_1 l_2 L} h_{l_3 l_4 L} \int r_1^2 dr_1 \int r_2^2 dr_2 F_L(r_1, r_2) \alpha_{l_1}(r_1) \beta_{l_2}(r_1) \alpha_{l_3}(r_2) \beta_{l_4}(r_2) \\ + g_{NL} h_{l_1 l_2 L} h_{l_3 l_4 L} \int r^2 dr \beta_{l_2}(r) \beta_{l_4}(r) [\mu_{l_1}(r) \beta_{l_3}(r) + \mu_{l_3}(r) \beta_{l_1}(r)]. \quad (39)$$

The expression of the CMB trispectrum in terms of the reduced trispectrum is given in equation (A1).

For detailed descriptions involving polarization maps, see Hu (2000), Komatsu & Spergel (2001), Hu & Okamoto (2002) and Kogo & Komatsu (2006). The CMB bispectrum, which describes departures from Gaussianity at the lowest level, can similarly be written as

$$B_{l_1 l_2 l_3} = 2f_{NL} h_{l_1 l_2 l_3} \int r^2 dr [\alpha_{l_1}(r) \beta_{l_2}(r) \beta_{l_3}(r) + \alpha_{l_2}(r) \beta_{l_3}(r) \beta_{l_1}(r) + \alpha_{l_3}(r) \beta_{l_2}(r) \beta_{l_1}(r)]. \quad (40)$$

We have defined the following form factor to simplify the display:

$$h_{l_1 l_2 l_3} = \sqrt{\frac{(2l_1 + 1)(2l_2 + 1)(2l_3 + 1)}{4\pi}} \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix}. \quad (41)$$

The extension to order beyond presented here to involve higher order Taylor coefficients may not be practically useful as the detector noise and the cosmic variance may prohibit any reasonable S/N.

5 NEAR OPTIMAL ESTIMATORS FOR THE TRISPECTRUM

In this section, we will develop two estimators for extraction of power spectra associated with the trispectrum (Hu 2000; Hu & Okamoto 2002), $\mathcal{K}_l^{3,1}$ and $\mathcal{K}_l^{2,2}$. These estimators are nearly optimized version of similar estimators considered in the previous section. The derivation here

parallels that of the previous section where unoptimized versions of these estimators were developed, which uses the PCL-type estimators. We will start by introducing four different fields, which are constructed from the temperature fields. These fields are defined over the observed part of the sky and are constructed using suitable weights to temperature harmonics. These weights are functions of the radial distance, $\alpha_l(r)$, $\beta_l(r)$ and $\mu_l(r)$, so the constructed fields are three-dimensional fields. This method follows the same technique as introduced by Komatsu et al. (2005):

$$A(r, \hat{\Omega}) = \sum_{lm} A_{lm} Y_{lm}(\hat{\Omega}); \quad B(r, \hat{\Omega}) = \sum_{lm} B_{lm} Y_{lm}(\hat{\Omega}); \quad M(r, \hat{\Omega}) = \sum_{lm} M_{lm} Y_{lm}(\hat{\Omega}); \quad (42)$$

$$A_{lm} = \frac{\alpha_{lm}}{C_l} a_{lm}; \quad B_{lm} = \frac{\beta_{lm}}{C_l} a_{lm}; \quad M_{lm} = \frac{\mu_{lm}}{C_l} a_{lm}. \quad (43)$$

We have absorbed the beam smoothing into the corresponding harmonic coefficients. In addition to the weighting functions, we will also need to define overlap integrals $F_L(r_1, r_2)$, which act as a kernel for cross-correlating fields at two different radial distances. Note that the overlap integral depends on the quantum number L :

$$F_L(r_1, r_2) = \frac{2}{\pi} \int k^2 dk P_{\Phi\Phi}(k) j_L(kr_1) j_L(kr_2). \quad (44)$$

In the following sections, we will use specific forms for the trispectra to construct an optimal estimator. Although the estimators developed here are specific to a given model, clearly, for any given model for the trispectra, we can obtain similar construction. The weighting of these harmonics makes the estimator a match-filtering one, which ensures maximum response when the trispectra obtained from the data match with those obtained with theoretical construct. Inverse variance weighting ensures that the estimator remains near optimal for a specific survey strategy.

We would like to emphasize here that an exact optimization of estimators for the trispectrum, based on the maximum-likelihood principle (see Appendix B for a detailed discussion), should use weights that include the full target trispectrum $T_{l_3 l_4}^{l_1 l_2}(L)$ (see equations A1 and A2 for definition). However, this is not possible using the map-based techniques that we will discuss in this section. Here the weights are constructed from the reduced trispectrum $\tau_{l_3 l_4}^{l_1 l_2}(L)$ (see equation 39 for definition). We use this approach to derive the following equation later as well as equations (61) and (68):

$$\left(\frac{S}{N}\right)^2 = \sum_L \sum_{l_1 > l_2 > l_3 > l_4} \frac{|T_{l_3 l_4}^{l_1 l_2}(L)|^2}{(2L+1)C_{l_1}C_{l_2}C_{l_3}C_{l_4}} \approx \sum_L \sum_{l_1 > l_2 > l_3 > l_4} \frac{|\tau_{l_3 l_4}^{l_1 l_2}(L)|^2}{(2L+1)C_{l_1}C_{l_2}C_{l_3}C_{l_4}}. \quad (45)$$

This particular approach of replacing the trispectrum T with the reduced trispectrum τ was used by Kogo & Komatsu (2006) to analyse the one-point estimator. It was initially introduced in the context of construction of optimal estimators for trispectra generated by lensing of CMB (Hu 2001). This is partly motivated by the fact that the additional terms that involve $6j$ symbols are computationally expensive (see Appendix A5 for more detailed discussions). They can, however, be evaluated using an approach based on the direct summation of modes that we present later in Section 7. The direct summation approach is exact and completely general; that is, it can be used to probe arbitrary target trispectra, primary or secondary. *A comparison of the approximate estimator presented here with the exact method is required to check the optimality of the estimators that are considered here, which remains unclear at this stage.*

5.1 Estimator for $\mathcal{K}^{(4)}$

We will start by defining a field $N(r_1, r_2)$, which is constructed from its harmonics N_{lm} that are in turn constructed from the functions $\alpha_l(r)$ and $\beta_l(r)$ that appear in the definition of the trispectrum (equation 39). The construction takes into account the overlap integral $F_l(r_1, r_2)$ and it is carried out by following the below-mentioned specific steps:

$$N_{lm}(r_1, r_2) = \int d\hat{\Omega} N(\hat{\Omega}, r_1, r_2) Y_{lm}^*(\hat{\Omega}); \quad N_{lm}^{AB}(r_1, r_2) = [F_l(r_1, r_2)]^{1/2} [AB]_{lm}(r_1); \quad (46)$$

$$[AB]_{lm}(r_1) = \sum_{l_1 m_1} \frac{\alpha_{l_1}(r_1)}{C_{l_1}} \frac{\beta_{l_2}(r_1)}{C_{l_2}} a_{l_1 m_1} a_{l_2 m_2} \int d\hat{\Omega} Y_{l_1 m_1}(\hat{\Omega}) Y_{l_2 m_2}(\hat{\Omega}) Y_{lm}^*(\hat{\Omega}); \quad (47)$$

$$N_{lm}^{AB}(r_1, r_2) = [F_l(r_2, r_1)]^{1/2} [AB]_{lm}(r_2) = N_{lm}(r_2, r_1). \quad (48)$$

The associated field $\bar{N}_{lm}(r_1, r_2)$ is constructed by changing the order of the radial variables r_1 and r_2 , and keeping in mind that $F_l(r_1, r_2)$ is a symmetric function of its arguments (equation 44). One-point estimators can now be computed directly in real space in terms of these fields and hence are simpler to compute when dealing with partial sky coverage in the presence of inhomogeneous noise. Using notations introduced above, we can write the one-point cumulant at fourth order as

$$\mathcal{K}^{(4)} = 4 f_{NL}^2 \int r_1^2 dr_1 \int r_2^2 dr_2 \int \frac{d\hat{\Omega}}{4\pi} \langle N^{AB}(\hat{\Omega}, r_1, r_2) \bar{N}^{AB}(\hat{\Omega}, r_1, r_2) \rangle + 2 g_{NL} \int r^2 dr \int \frac{d\hat{\Omega}}{4\pi} B^3(r, \hat{\Omega}) M(r, \hat{\Omega}), \quad (49)$$

which can be written in a compact form using the following notation:

$$\mathcal{K}^{(4)} = 4 f_{NL}^2 \int r_1^2 dr_1 \int r_2^2 dr_2 N^{(AB)}(\hat{\Omega}, r_1, r_2) \bar{N}^{(AB)}(\hat{\Omega}, r_1, r_2) + 2 g_{NL} \int r^2 dr \langle B^3(r, \hat{\Omega}) M(r, \hat{\Omega}) \rangle. \quad (50)$$

As expected there are two parts in the contribution. The first part depends on two radial directions through the overlap integral $F_L(r_1, r_2)$; the second is much simpler and just contains one line-of-sight integration. The amplitude of the first term depends on f_{NL}^2 and the second term is proportional to g_{NL} . Typically, they contribute equally to the resulting estimate. Expressing $\mathcal{K}^{(4)}$ in harmonic domain, it is relatively easy to show that

$$\mathcal{K}^{(4)} = \sum_l \sum_{l_i} \frac{1}{2l+1} \frac{\tau_{l_3 l_4}^{l_1 l_2}(l) T_{l_3 l_4}^{l_1 l_2}(l)}{C_{l_1} C_{l_2} C_{l_3} C_{l_4}}. \quad (51)$$

This allows us to write the S/N for the one-point trispectrum estimator as given in equation (45).

Several comments are in order. The expression in equation (45) is an approximation that was introduced by Kogo & Komatsu (2006) in their study. This is partly motivated by the fact that numerical evaluation of $6j$ symbols is relatively cumbersome. The construction of $\mathcal{K}^{(4)}$ that we have presented takes into account the reduced trispectrum $\tau_{l_3 l_4}^{l_1 l_2}(l)$. However, we are able to show that several other terms can be incorporated using a map-based approach, which we will present in Appendix A. If we adhere to the approach given in Kogo & Komatsu (2006), which replaces the trispectrum $T_{l_3 l_4}^{l_1 l_2}(l)$ with the reduced trispectrum $\tau_{l_3 l_4}^{l_1 l_2}$ and ignore the cross-terms, which involve the $6j$ symbols, that are subdominant, then we will recover the Kogo & Komatsu (2006) estimator from the estimator derived above (equation 51). To restrict the sum on the upper *triangular* part of the four-dimensional matrix, we need to remember that $\sum_{l_i} = 4! \sum_{l_1 > l_2 > l_3 > l_4}$ and hence $\mathcal{K}^{(4)} = 24(\frac{S}{N})^2$. Next, we will introduce the two-point estimators $\mathcal{K}_l^{(3,1)}$ and $\mathcal{K}_l^{(2,2)}$, and establish their connection to the one-point estimator introduced here.

Needless to say that it is indeed possible to add the terms that we have ignored by direct summation of contributing modes. This is clearly computationally demanding and even in case of factorizable models, it is not possible to devise a simple map-based method adopted here.

5.2 Estimator for $\mathcal{K}_l^{(3,1)}$

Moving beyond the one-point cumulants, we can construct the estimators of the two power spectra, which we discussed before, $C_l^{(3,1)}$ and $C_l^{(2,2)}$. The corresponding optimized versions can be constructed by cross-correlating the fields constructed suitably from weighted maps $A(r)$ and $B(r)$.

Clearly, in the first case, the harmonics depend on two radial distances r_1 and r_2 for any given angular direction. We start by constructing a field $C(r, \hat{\Omega}) = A(r, \hat{\Omega})B(r, \hat{\Omega})$. In harmonic domain, the harmonic components are related by the following expression:

$$C_{LM}(r_1) = \int d\hat{\Omega} A(r_1, \hat{\Omega}) B(r_1, \hat{\Omega}) Y_{LM}^*(\hat{\Omega}) d\hat{\Omega}; \quad C_{LM}(r_1) = \sum_M (-1)^M \frac{\alpha_{l_1}(r_1)}{C_{l_1}} \frac{\beta_{l_2}(r_1)}{C_{l_2}} \mathcal{G}_{l_1 l_1 L}^{m_1 m_2 - M} a_{l_1 m_1} a_{l_2 m_2}. \quad (52)$$

By suitably weighting the harmonic coefficients $C_{LM}(r_1)$, we construct a new harmonics $C_{LM}(r_2)$ by the following expressions:

$$C'(r_1, r_2, \hat{\Omega}) = \sum_{LM} C'_{LM}(r_1, r_2) Y_{LM}^*(\hat{\Omega}) = \sum_{LM} (-1)^M F_L(r_1, r_2) C_{LM}(r_1) Y_{L-M}(\hat{\Omega}); \quad (53)$$

$$C'_{LM}(r_1, r_2) = F_L(r_1, r_2) C_{LM}(r_1, r_2).$$

Projecting the harmonics $C'_{LM}(r_1, r_2)$, we construct a map $C'(r_1, r_2, \hat{\Omega})$. Next, we consider the product map $D(r_1, r_2, \hat{\Omega}) = C'(r_1, r_2, \hat{\Omega})A(r_2, \hat{\Omega})$. This map depends on two radial distances r_1 and r_2 . In Fourier domain, the harmonics of D are expressed by the following relation:

$$D(r_1, r_2)_{lm} \equiv \int D(r_1, r_2) Y_{lm}^* d\hat{\Omega} = \sum_{LM} \sum_{l_3 m_3} C'_{LM}(r_1, r_2) \frac{\alpha_{l_3}(r_2)}{C_{l_3}} (-1)^m \mathcal{G}_{M m_3 - m}^{L l_3 l}. \quad (54)$$

Next, we compute the cross-power spectra $D(\hat{\Omega}, r_1, r_2)$ and $B(\hat{\Omega}, r_2)$. We will denote this with $\mathcal{J}_l^{A^2 B, A}(r_2)$, which depends only on the radial distance r_2 :

$$\mathcal{J}_l^{A^2 B, A}(r_1, r_2) = \frac{1}{2l+1} \sum_m \text{Real} [D(r_1, r_2)_{lm} B(r_2)_{lm}^*]. \quad (55)$$

The construction for the second term is simpler. We start by decomposing the real-space product $A(r, \hat{\Omega})B^2(r, \hat{\Omega})$ and $M(r, \hat{\Omega})$ in harmonic space. There is only one radial distance involved in both these terms:

$$MB^2(r)_{lm} = \int [MB^2(r, \hat{\Omega})] Y_{lm}^*(\hat{\Omega}) d\hat{\Omega}; \quad B(r)_{lm} = \int B(r) Y_{lm}^*(\hat{\Omega}) d\hat{\Omega}. \quad (56)$$

Finally, the line-of-sight integral, which involves two overlapping contributions through the weighting kernels for the first term and only one for the second, gives the required estimator:

$$\hat{\mathcal{K}}_l^{(3,1)} = 4f_{nl}^2 \int r_1^2 dr_1 \int r_2^2 dr_2 \mathcal{J}_l^{A^2 B, A}(r_1, r_2) + 2g_{nl} \int r^2 dr \mathcal{L}_l^{MB^2, B}(r). \quad (57)$$

Next, we show that the construction described above reduces to an optimum estimator for the power spectrum associated with the trispectrum. The harmonics associated with the product field $A(r_1)B(r_1)A(r_2)$ can be expressed in terms of the functions $\alpha(r)$ and $\beta(r)$ as

$$D(r_1, r_2)_{lm} = \sum_{LM} (-1)^M \sum_{l_m, l_i, m_i} (-1)^m a_{l_1 m_1} a_{l_2 m_2} a_{l_3 m_3} F_L(r_1, r_2) \frac{\alpha_{l_1}(r_1)}{C_{l_1}} \frac{\beta_{l_2}(r_1)}{C_{l_2}} \frac{\alpha_{l_3}(r_2)}{C_{l_3}} \mathcal{G}_{m_1 m_2 - M}^{l_1 l_2 L} \mathcal{G}_{M m_3 - m}^{L l_3 l}. \quad (58)$$

The cross-power spectra $\mathcal{J}_l^{AB^2,A}(r_1, r_2)$ can be simplified in terms of the following expression:

$$\mathcal{J}_l^{A^2B,B}(r_1, r_2) = \frac{1}{2l+1} \sum_{LM} (-1)^M \sum_m \left\{ F_L(r_1, r_2) \frac{\alpha_{l_1}(r_1)}{C_{l_1}} \frac{\beta_{l_2}(r_1)}{C_{l_2}} \frac{\alpha_{l_3}(r_2)}{C_{l_3}} \frac{\beta_{l_4}(r_2)}{C_{l_4}} \right\} \langle a_{l_1 m_1} a_{l_2 m_2} a_{l_3 m_3} a_{l_4 m_4}^* \rangle \mathcal{G}_{m_1 m_2 - m}^{l_1 l_2 L} \mathcal{G}_{m_3 m_4 - m}^{l_3 l_4 L}, \quad (59)$$

where the Gaunt integral $\mathcal{G}_{m_1 m_2 m_3}^{l_1 l_2 l_3}$ describing the overlap integral involving three spherical harmonics is defined in equation (C5). The second term can be treated in an analogous way and takes the following form:

$$\mathcal{L}_l^{MB^2,B}(r) = \frac{1}{2l+1} \sum_{LM} (-1)^M \sum_m (-1)^m \left\{ \frac{\mu_{l_1}(r)}{C_{l_1}} \frac{\beta_{l_2}(r)}{C_{l_2}} \frac{\beta_{l_3}(r)}{C_{l_3}} \frac{\beta_{l_4}(r)}{C_{l_4}} \right\} \langle a_{l_1 m_1} a_{l_2 m_2} a_{l_3 m_3} a_{l_4 m_4}^* \rangle \mathcal{G}_{m_1 m_2 - m}^{l_1 l_2 L} \mathcal{G}_{m_3 m_4 - m}^{l_3 l_4 L}. \quad (60)$$

Finally, on combining these terms as in equation (57), we recover the following expression:

$$\hat{\mathcal{K}}_l^{(3,1)} = \frac{1}{2l+1} \sum_{l_1 l_2 l_3} \sum_L \frac{1}{(2L+1)} \frac{1}{C_{l_1} C_{l_2} C_{l_3} C_L} \tau_{l_1 l_2}^{l_1 l_2 L} [L] T_{l_3 l_4}^{l_1 l_2 L} [L]. \quad (61)$$

The estimator $\mathcal{K}_l^{(3,1)}$ linearly depends on both f_{NL}^2 and g_{NL} . In principle, we can use the estimate of f_{NL} from a bispectrum analysis as a prior or we can use the estimators $\mathcal{S}_l^{(2,1)}$, $\mathcal{K}_l^{(3,1)}$ and $\mathcal{K}_l^{(3,1)}$ to put joint constraints on f_{NL} and g_{NL} . Computational evaluation of either of the power spectra clearly will be more involved as a double integral corresponding to two radial directions needs to be evaluated. Given the low S/N associated with these power spectra, binning will be essential.

5.3 Estimator for $\mathcal{K}_l^{(2,2)}$

In an analogous way, the other power spectra associated with the trispectra can be optimized by the following construction. We start by taking the harmonic transform of the product field $A(r, \hat{\Omega})B(r, \hat{\Omega})$ evaluated at the same line-of-sight distance r :

$$A(r, \hat{\Omega})B(r, \hat{\Omega})|_{lm} = \int A(r)B(r)Y_{lm}^*(\hat{\Omega})d\hat{\Omega}, \quad B(r, \hat{\Omega})M(r, \hat{\Omega})|_{lm} = \int B(r)M(r)Y_{lm}^*(\hat{\Omega})d\hat{\Omega}, \quad (62)$$

and contract it with its counterpart at a different distance. The corresponding power spectrum (which is a function of these two line-of-sight distances r_1 and r_2) has the first term

$$\mathcal{J}_l^{AB,AB}(r_1, r_2) = \frac{1}{2l+1} \sum_m F_l(r_1, r_2) A(r_1, \hat{\Omega})B(r_1, \hat{\Omega})|_{lm} A(r_2, \hat{\Omega})B(r_2, \hat{\Omega})|_{lm}^*. \quad (63)$$

Similarly, the second part of the contribution can be constructed by cross-correlating the product of three-dimensional fields $A(\hat{\Omega}, r_1)B(\hat{\Omega}, r_1)$ and $B(\hat{\Omega}, r_2)M(\hat{\Omega}, r_2)$ evaluated at different distances r_1 and r_2 :

$$\mathcal{L}_l^{BB,BM}(r) = \frac{1}{2l+1} \sum_m \text{Real} [B(r, \hat{\Omega})B(r, \hat{\Omega})|_{lm} B(r, \hat{\Omega})M(r, \hat{\Omega})|_{lm}^*]. \quad (64)$$

Finally, the estimator is constructed as (see Appendix A for more detailed discussion):

$$\hat{\mathcal{K}}_l^{(2,2)} = 4f_{nl}^2 \int r_1^2 dr_1 \int r_2^2 dr_2 \mathcal{J}_l^{AB,AB}(r_1, r_2) + 2g_{nl} \int r^2 dr \mathcal{L}_l^{BB,BM}(r). \quad (65)$$

To see they do correspond to an optimum estimator, we use the harmonic expansions and follow the same procedure as outlined before:

$$\mathcal{L}_l^{BB,BM}(r) = \frac{1}{2l+1} \sum_m (-1)^m \sum_{l_1 m_1} \left\{ \frac{\beta_{l_1}(r)}{C_{l_1}} \frac{\beta_{l_2}(r)}{C_{l_2}} \frac{\beta_{l_3}(r)}{C_{l_3}} \frac{\mu_{l_4}(r)}{C_{l_4}} \right\} \langle a_{l_1 m_1} a_{l_2 m_2} a_{l_3 m_3}^* a_{l_4 m_4}^* \rangle \mathcal{G}_{m_1 m_2 - m}^{l_1 l_2 l} \mathcal{G}_{m_3 m_4 - m}^{l_3 l_4 l}; \quad (66)$$

$$\mathcal{J}_l^{AB,AB}(r_1, r_2) = \frac{1}{2l+1} \sum_m (-1)^m \sum_{m_i} \left\{ F_l(r_1, r_2) \frac{\alpha_{l_1}(r_1)}{C_{l_1}} \frac{\beta_{l_2}(r_1)}{C_{l_2}} \frac{\alpha_{l_3}(r_2)}{C_{l_3}} \frac{\beta_{l_4}(r_2)}{C_{l_4}} \right\} \langle a_{l_1 m_1} a_{l_2 m_2} a_{l_3 m_3}^* a_{l_4 m_4}^* \rangle \mathcal{G}_{m_1 m_2 - m}^{l_1 l_2 l} \mathcal{G}_{m_3 m_4 - m}^{l_3 l_4 l}. \quad (67)$$

Here we notice that $\mathcal{J}_l^{AB,AB}(r_1, r_2)$ is invariant under exchange of r_1 and r_2 but $\mathcal{J}_l^{AB,BM}(r_1, r_2)$ is not. Finally, joining the various contributions to construct the final estimator, as given in equation (65), which involves a line-of-sight integration, we get

$$\hat{\mathcal{K}}_l^{(2,2)} = \frac{1}{2l+1} \sum_{l_i} \frac{1}{(2l+1)} \frac{1}{C_{l_1} C_{l_2} C_{l_3} C_{l_4}} \tau_{l_1 l_2}^{l_1 l_2 l} (l) T_{l_3 l_4}^{l_1 l_2 l} (l). \quad (68)$$

The pre-factors associated with f_{NL}^2 and g_{NL} are different in the linear combinations $\mathcal{K}_l^{(2,2)}$ and $\mathcal{K}_l^{(3,1)}$, and hence even without using information from third order we can estimate both from fourth order alone. In our derivation for these power spectra, we have replaced the full trispectrum with a reduced one; such an approximation is also used for analysis of the trispectrum generated due to effect of weak lensing of CMB.

Figs 1 and 2 show the primordial $\mathcal{K}_l^{(2,2)}$ and $\mathcal{K}_l^{(3,2)}$ for the *WMAP5* best-fitting cosmological parameters (Dunkley et al. 2009), integrated over a range of 500 Mpc around recombination and shown as a function of the harmonic number l . The computations of \mathcal{K}_l typically scale as l_{\max}^3 with resolution, which makes it quite expensive for high-resolution studies. The computations are largely dominated by computations of $3j$ symbols. For a given configuration number of non-zero $3j$ symbols for which the computations are required, they roughly scale as l_{\max}^3 , which explains the scaling. For more details about noise and beam, see Smidt et al. (2009).

The unbiased version of $\mathcal{K}_l^{(2,2)}$ has been used in the context of studying lensing effects on CMB maps (Cooray & Kesden 2003). While cross-correlational analysis can be helpful for detection of lensing on CMB maps for internal detection involving only CMB maps, an analysis at the trispectrum level is necessary.

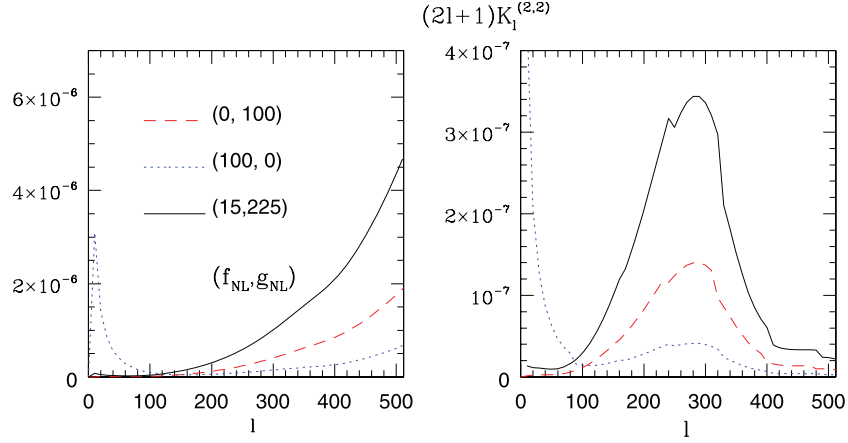


Figure 1. The trispectrum-related power spectrum $\mathcal{K}_l^{(2,2)}$ is plotted as a function of the angular scale l . The left-hand panel is for a noise-free ideal all-sky experiment. The right-hand panel corresponds to *WMAP* V-band noise. Various curves correspond to a specific parameter combination of $(f_{\text{NL}}, g_{\text{NL}})$ as indicated (see text for details).

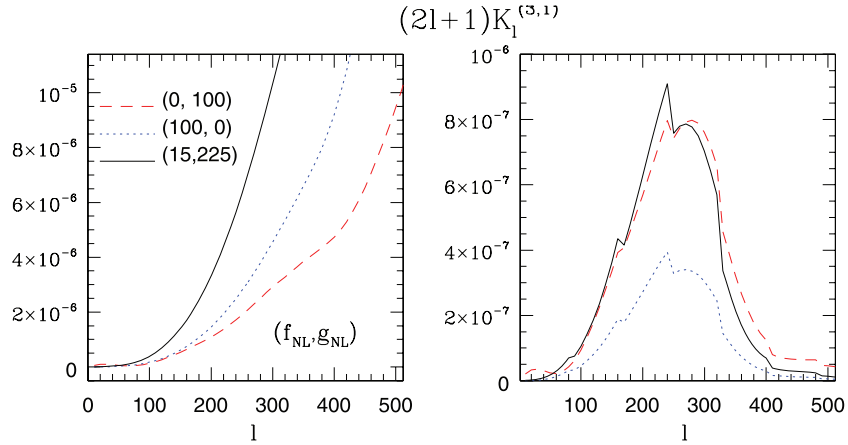


Figure 2. Same as Fig. 1, but for the trispectrum-related power spectrum $\mathcal{K}_l^{(3,1)}$ plotted as a function of the angular scale l for ideal (left-hand panel) and *WMAP* V-band noise characteristics.

5.4 Linking various estimators

The one-point estimators can be expressed as a summation over all values of l of the estimators $\mathcal{K}_l^{(3,1)}$ or $\mathcal{K}_l^{(2,2)}$. Therefore, the corresponding optimized one-point estimators $\hat{\mathcal{K}}^{(4)}$ can be written as

$$\hat{\mathcal{K}}^{(4)} = \sum_{l_i L} \frac{1}{(2L+1)} \frac{\tau_{l_3 l_4}^{l_1 l_2}(L) \hat{T}_{l_1 l_2}^{l_3 l_4}(L)}{C_{l_1} C_{l_2} C_{l_3} C_{l_4}}. \quad (69)$$

Here $\hat{T}_{l_1 l_2}^{l_3 l_4}(L)$ denotes the direct estimator from the harmonic transforms and $T_{l_1 l_2}^{l_3 l_4}(L)$ acts as weights, which are constructed using the optimization function discussed above. Similarly, at the two-point level, the corresponding power spectra can be written as

$$\hat{\mathcal{K}}_l^{(2,2)} = \frac{1}{(2l+1)} \sum_{l_i} \frac{1}{(2l+1)} \frac{\tau_{l_3 l_4}^{l_1 l_2}(l) \hat{T}_{l_3 l_4}^{l_1 l_2}(l)}{C_{l_1} C_{l_2} C_{l_3} C_{l_4}}; \quad \hat{\mathcal{K}}_l^{(3,1)} = \frac{1}{(2l+1)} \sum_{l_i L} \frac{1}{(2L+1)} \frac{\tau_{l_3 l}^{l_1 l_2}(L) \hat{T}_{l_3 l}^{l_1 l_2}(L)}{C_{l_1} C_{l_2} C_{l_3} C_l}. \quad (70)$$

Each contribution from a specific configuration formed by various values of l_i and L is weighted by the corresponding C_l to make the estimator optimal. For computation of the variances, the fields are, however, considered as Gaussian, which should be a good approximation as the fields are expected to be close to Gaussian. Note that the values of C_l here take contributions from both the signal and the noise terms, that is, $C_l = C_l^S + C_l^N$, where C_l^S is just the theoretical expectation for primordial perturbations.

Both $\mathcal{K}_l^{(2,2)}$ and $\mathcal{K}_l^{(3,1)}$ involve both parameters f_{NL} and g_{NL} and can be used for a joint analysis, along with $\mathcal{S}_l^{(2,1)}$, to put constraints from realistic data. It is easy to check that the following relationship holds:

$$\hat{\mathcal{K}}^{(4)} = \sum_l (2l+1) \hat{\mathcal{K}}_l^{(2,2)} = \sum_l (2l+1) \hat{\mathcal{K}}_l^{(3,1)}. \quad (71)$$

These results therefore generalize the results obtained in Munshi & Heavens (2010) in the context of bispectral analysis.

It is important to realize that though we have focused on a very specific model for the trispectrum, it is applicable to any other trispectrum as long as a factorization is available.

5.5 Subtracting the Gaussian or disconnected contributions

In estimating the trispectrum, we need to subtract out the disconnected or Gaussian parts (Hu 2000; Hu & Okamoto 2002). To do this, we follow the same procedure but replacing the simulated non-Gaussian maps with their Gaussian counterparts. Both maps should be constructed to have the same power spectrum and identical noise. If the noise is Gaussian, then it will only contribute to the disconnected part. For construction of an estimator, which is noise-subtracted, we need to follow the same procedure as above by constructing Gaussian maps $A^G(r, \hat{\Omega})$, $B^G(r, \hat{\Omega})$, etc.

$$A^G(\hat{\Omega}, r) = \sum_{lm} A_{lm}^G Y_{lm}(\hat{\Omega}); \quad B^G(\hat{\Omega}, r) = \sum_{lm} B_{lm}^G Y_{lm}(\hat{\Omega}); \quad M^G(\hat{\Omega}, r) = \sum_{lm} M_{lm}^G Y_{lm}(\hat{\Omega});$$

$$A_{lm}^G = \frac{\alpha_{lm}}{C_l} a_{lm}^G; \quad B_{lm}^G = \frac{\beta_{lm}}{C_l} a_{lm}^G; \quad M_{lm}^G = \frac{\mu_{lm}}{C_l} a_{lm}^G. \quad (72)$$

We illustrate this using $\mathcal{K}_l^{(2,2)}$; the analysis is very similar for the other estimator. We start by replacing the quantities $\mathcal{I}_l^{AB,AB}(r_1, r_2)$ and $\mathcal{L}_l^{AB,AB}(r_1, r_2)$ by their Gaussian counterparts, $\mathcal{P}_l^{A^G B^G, A^G B^G}(r_1, r_2)$ and $\mathcal{R}_l^{A^G B^G, B^G M^G}(r)$, which are constructed in an exactly the same manner, simply replacing the observed map with the Gaussian maps:

$$\mathcal{P}_l^{A^G B^G, A^G B^G}(r_1, r_2) = \frac{1}{2l+1} \sum_m \sum_{m_i} F_l(r_1, r_2) \text{Real} [A^G(r_1, \hat{\Omega}) B^G(r_1, \hat{\Omega})_{lm} A^G(r_2, \hat{\Omega}) B^G(r_2, \hat{\Omega})_{lm}^*];$$

$$\mathcal{P}_l^{(A^G B^G, A^G B^G)}(r_1, r_2) = \frac{1}{2l+1} \sum_{LM} (-1)^M \sum_m \left\{ F_l(r_1, r_2) \frac{\alpha_{l_1}(r_1)}{C_{l_1}} \frac{\beta_{l_2}(r_1)}{C_{l_2}} \frac{\alpha_{l_3}(r_2)}{C_{l_3}} \frac{\beta_{l_4}(r_2)}{C_{l_4}} \right\} \langle a_{l_1 m_1}^G a_{l_2 m_2}^G a_{l_3 m_3}^G a_{l_4 m_4}^G \rangle \mathcal{G}_{l_1 l_2 l}^{m_1 m_2 m} \mathcal{G}_{l_3 l_4 l}^{m_3 m_4 m}. \quad (73)$$

These quantities are then used for the construction of an estimator, which, in practice, aims to estimate the Gaussian contributions to the total trispectra:

$$\mathcal{R}_l^{A^G B^G, B^G M^G}(r) = \frac{1}{2l+1} \sum_m \text{Real} [B^G(r, \hat{\Omega}) B^G(r, \hat{\Omega})_{lm} B^G(r, \hat{\Omega}) M^G(r, \hat{\Omega})_{lm}^*];$$

$$\mathcal{R}_l^{(A^G B^G, B^G M^G)}(r) = \frac{1}{2l+1} \sum_m (-1)^m \sum_{l_i m_i} \left\{ \frac{\beta_{l_1}(r)}{C_{l_1}} \frac{\beta_{l_2}(r)}{C_{l_2}} \frac{\beta_{l_3}(r)}{C_{l_3}} \frac{\mu_{l_4}(r)}{C_{l_4}} \right\} \langle a_{l_1 m_1}^G a_{l_2 m_2}^G a_{l_3 m_3}^G a_{l_4 m_4}^G \rangle \mathcal{G}_{l_1 l_2 l}^{m_1 m_2 m} \mathcal{G}_{l_3 l_4 l}^{m_3 m_4 m}. \quad (74)$$

As before we combine these quantities to form the weighted Gaussian part of the contribution to the trispectrum:

$$\mathcal{G}_l^{(2,2)} = 4f_{nl}^2 \int r_1^2 dr_1 \int r_2^2 dr_2 \mathcal{P}_l^{A^G B^G, A^G B^G}(r_1, r_2) + 2g_{NL} \int r^2 dr \mathcal{R}_l^{A^G B^G, B^G M^G}(r) = \frac{1}{(2l+1)^2} \sum_{l_i} \frac{\tau_{l_3 l_4}^{l_1 l_2}(l)}{C_{l_1} C_{l_2} C_{l_3} C_{l_4}} G_{l_3 l_4}^{l_1 l_2}(l). \quad (75)$$

Subtracting the Gaussian contribution from the total estimator, we have

$$\hat{\mathcal{K}}_l^{(2,2)} = \mathcal{K}_l^{(2,2)} - \mathcal{G}_l^{(2,2)} = \frac{1}{(2l+1)^2} \sum_{l_i} \frac{1}{C_{l_1} C_{l_2} C_{l_3} C_{l_4}} \tau_{l_3 l_4}^{l_1 l_2}(l) \left\{ \hat{\mathcal{T}}_{l_3 l_4}^{l_1 l_2}(l) - G_{l_3 l_4}^{l_1 l_2}(l) \right\}. \quad (76)$$

A very similar calculation for the other fourth-order estimator $\mathcal{G}_l^{3,1}$ provides an identical result. After subtraction of the Gaussian contribution, we have

$$\hat{\mathcal{K}}_l^{(3,1)} = \mathcal{K}_l^{(3,1)} - \mathcal{G}_l^{(3,1)} = \frac{1}{(2l+1)} \sum_{l_i} \sum_L \frac{1}{(2L+1)} \frac{1}{C_{l_1} C_{l_2} C_{l_3} C_l} \tau_{l_3 l_4}^{l_1 l_2}(L) \left\{ \hat{\mathcal{T}}_{l_3 l}^{l_1 l_2}(L) - G_{l_3 l}^{l_1 l_2}(L) \right\}. \quad (77)$$

The corresponding one-point collapsed estimator has the following form and the relationship between the various estimators remains unchanged:

$$\hat{\mathcal{K}}_l^{(4)} = \sum_{l_i} \frac{1}{(2l+1)} \frac{1}{C_{l_1} C_{l_2} C_{l_3} C_{l_4}} \tau_{l_3 l_4}^{l_1 l_2}(l) \left\{ \hat{\mathcal{T}}_{l_3 l_4}^{l_1 l_2}(l) - G_{l_3 l_4}^{l_1 l_2}(l) \right\}. \quad (78)$$

Notice that we have constructed the Gaussian term from Monte Carlo (MC) averaging that uses Gaussian simulations. In principle, it may also be constructed from analytical modelling.

In the next section, we consider partial sky coverage and the resulting corrections to the Gaussian and non-Gaussian terms in each of the estimators.

6 PARTIAL SKY COVERAGE AND OPTIMIZED ESTIMATORS

The terms that are needed for correcting the effect of finite sky coverage and inhomogeneous noise are listed below. These corrections are incorporated by using MC simulations of noise realizations (Creminelli 2003; Babich & Zaldarriaga 2004; Babich, Creminelli & Zaldarriaga 2004; Babich 2005; Creminelli et al. 2006, 2007a,b), whereas in case of bispectral analysis, it is just the linear terms, which are needed for corrections, and for the case of trispectral analysis, there are only quadratic terms. We will treat the general case in the following sections, but first we present results for the simpler case of homogeneous noise and for high wavenumbers, where the density of uncorrelated states is modified by inclusion of the fraction of sky observed, f_{sky} .

In a recent paper, Yadav et al. (2008) developed a novel prescription for the construction of correction terms for various estimators in the absence of spherical symmetry. This method was shown to work for the analysis of a bispectrum (skewness and skew spectrum) for both

local and equilateral models of non-Gaussianity. This procedure depends on using MC simulations to correct for the effect of mask as well as inhomogeneous noise. The bispectrum, which is defined as $\langle xyz \rangle$ for the three suitably filtered fields, x , y and z , can be decomposed using Wick's theorem as $\langle x \rangle \langle yz \rangle + \langle y \rangle \langle xz \rangle + \langle z \rangle \langle xy \rangle$. Here the angular brackets denote MC averages. Following Yadav et al. (2008), the correction terms can now be constructed by replacing the MC average from the single maps, that is, $x \langle yz \rangle + y \langle xz \rangle + z \langle xy \rangle$. These corrections are linear in the input field variables x , y and z . The above procedure can be generalized for the construction of correction terms for the trispectrum. We will devise a method that can be applied both to the non-Gaussian (connected) terms and to the Gaussian (disconnected) contributions that need to be subtracted out. The four-point average can similarly be decomposed using Wick's theorem: $\langle wxyz \rangle = (\langle w \rangle \langle xyz \rangle + \text{cyclic permutation}) + (\langle wx \rangle \langle yz \rangle + \text{cyclic permutation})$. The construction of correction terms can now be done by applying the same technique. The first set of terms are recovered by removing the MC average from the single maps, thereby generating terms such as $w \langle xyz \rangle$. These terms depend on the bispectrum of the relevant field variables. We will ignore them as is the norm in any construction of optimal trispectrum estimators. The second type of terms consists of three different terms, that is, $\langle wx \rangle \langle yz \rangle + \langle wy \rangle \langle xz \rangle + \langle wz \rangle \langle xy \rangle$. To construct the correction to these terms, we have to replace each MC average of product of two fields with a product without the averaging. Following this procedure, we will generate two terms from each individual term, for example, $\langle wx \rangle \langle yz \rangle$ will be replaced by $wx \langle yz \rangle + \langle wx \rangle yz$. Hence, there will be a total of six correction terms for each of our estimators. We will see later in Appendix A that the same correction terms can be recovered by maximization of probability distribution function, again by ignoring the bispectrum.

In what follows, we will list correction terms for each of the estimators introduced before.

6.1 Corrective terms for the estimator $\mathcal{K}_l^{(3,1)}$ in the absence of spherical symmetry

We list below the corrections to the individual contributions:

$$\hat{\mathcal{J}}_l^{A_1 B_1 A_2 B_2} = \frac{1}{f_{\text{sky}}} \left[\tilde{\mathcal{J}}_l^{A_1 B_1 A_2 B_2} - \mathcal{J}_l^{\text{corr}} \right]; \quad (79)$$

$$\mathcal{J}_l^{\text{corr}} = \frac{1}{f_{\text{sky}}} \left[\mathcal{J}_l^{(A_1 B_1) A_2 B_2} + \mathcal{J}_l^{(A_1 A_2) B_1 B_2} + \mathcal{J}_l^{(B_1 A_2) A_1 B_2} + \mathcal{J}_l^{A_1 B_1 (A_2 B_2)} + \mathcal{J}_l^{A_1 A_2 (B_1 B_2)} + \mathcal{J}_l^{B_1 A_2 (A_1 B_2)} \right]. \quad (80)$$

The expressions are similar for the other terms that depend on only one radial distance:

$$\hat{\mathcal{L}}_l^{B^2 M, B} = \frac{1}{f_{\text{sky}}} \left[\tilde{\mathcal{L}}_l^{M B^2, B} - \mathcal{L}_l^{\text{corr}} \right]; \quad (81)$$

$$\mathcal{L}_l^{\text{corr}} = \frac{1}{f_{\text{sky}}} \left[2\mathcal{L}_l^{M B (B, B)} + \mathcal{L}_l^{B^2 (M, B)} + 2\mathcal{L}_l^{B (M B), B} + \mathcal{L}_l^{M (B^2), B} \right]. \quad (82)$$

To simplify the presentation, we have used the symbol $A(r_1, \hat{\Omega}) = A_1$; $A(r, \hat{\Omega}) = A$ and so on. Essentially, we can see that there are terms which are linear in the input harmonics and terms which are quadratic in the input harmonics. The terms which are linear are also proportional to the bispectrum of the remaining three-dimensional fields, which are being averaged. On the other hand, the pre-factors for quadratic terms are three-dimensional correlation functions of the remaining two fields. Finally, putting all these expressions together, we can write

$$\tilde{\mathcal{K}}_l^{(3,1)} = 4f_{NL}^2 \int r_1^2 dr_1 \int r_2^2 dr_2 \tilde{\mathcal{J}}_l^{A^2 B, B}(r_1, r_2) + 2g_{NL} \int r^2 dr \tilde{\mathcal{L}}_l^{M B^2, B}(r). \quad (83)$$

From a computational point of view, clearly, the overlap integral $F_L(r_1, r_2)$ will be expensive and may determine to what resolution ultimately these direct techniques can be implemented. Use of these techniques directly involving MC numerical simulations will be dealt with in a separate paper (Smidt et al., in preparation). To what extent the linear and quadratic terms are important in each of these contributions can only be decided by testing against simulation.

6.2 Corrective terms for the estimator $\mathcal{K}_l^{(2,2)}$ in the absence of spherical symmetry

The unbiased estimator for the other estimator can be constructed in a similar manner. As before, these are terms which are quadratic in input harmonics with a pre-factor proportional to terms involving cross-correlation or variance of various combinations of three-dimensional fields:

$$\hat{\mathcal{J}}_l^{A_1 B_1, A_2 B_2} = \frac{1}{f_{\text{sky}}} \left[\tilde{\mathcal{J}}_l^{A_1 B_1, A_2 B_2} - \mathcal{J}_l^{\text{corr}} \right]; \quad (84)$$

$$\mathcal{J}_l^{\text{corr}} = \frac{1}{f_{\text{sky}}} \left[\mathcal{J}_l^{A_1 B_1, (A_2 B_2)} + \mathcal{J}_l^{(A_1 B_1), A_2 B_2} + \mathcal{J}_l^{A_1 (B_1, B_2) A_2} + \mathcal{J}_l^{B_1 (A_1, B_2) A_2} + \mathcal{J}_l^{B_1 (A_1, A_2) B_2} + \mathcal{J}_l^{A_1 (B_1, A_2) B_2} \right]. \quad (85)$$

The terms such as $\mathcal{K}_l^{AB, BM}(r_1, r_2)$ can be constructed in a very similar way. We display the term $\mathcal{K}_l^{AB^2, A}(r_1, r_2)$ with all its corrections included:

$$\hat{\mathcal{L}}_l^{B^2, BM} = \frac{1}{f_{\text{sky}}} \left[\tilde{\mathcal{L}}_l^{B^2, BM} - \mathcal{L}_l^{\text{corr}} \right] \quad (86)$$

$$\mathcal{L}_l^{\text{corr}} = \frac{1}{f_{\text{sky}}} \left[\mathcal{L}_l^{(B^2), BM} + 2\mathcal{L}_l^{B (B, M) B} + \mathcal{K}_l^{B^2, (BM)} + 2\mathcal{K}_l^{B (B, B) M} \right]. \quad (87)$$

The correction terms to the Gaussian contribution can likewise be derived using Gaussian simulations. The techniques developed here using MC maps are known to reduce the scatter and can greatly simplify the estimation of non-Gaussianity. This can be useful, as fully optimal analysis with inverse variance weighting, which treats mode–mode coupling completely, may only be possible on low-resolution maps.

6.3 Corrective terms for the estimator $\mathcal{K}^{(4)}$ in the absence of spherical symmetry

The corrections to the optimized one-point fourth-order cumulant can also be analysed in a very similar manner. It is expected that higher order cumulants will be more affected by partial sky coverage and loss of spherical symmetry because of inhomogeneous noise:

$$\hat{\mathcal{K}}^{(4)} = \frac{1}{f_{\text{sky}}} [\tilde{\mathcal{K}}^{(4)} - K^{\text{corr}}]. \quad (88)$$

The linear and quadratic terms can be expressed in terms of MC averages. We list terms which involve the overlap integral and the one with single line-of-sight integration:

$$K^{\text{corr}} = 4f_{NL}^2 \int r_1^2 dr_1 \int r_2^2 dr_2 \{ N^{A_1(B_1) \tilde{N}^{A_2)B_2} + N^{B_1(A_1) N^{A_2)B_2} + N^{B_1(A_1) \tilde{N}^{B_2)A_2} + N^{A_1(B_1) \tilde{N}^{B_2)A_2} \} \\ + 2g_{NL} \int r^2 dr \{ 3B \langle B^2 M \rangle + M \langle B^3 \rangle \}. \quad (89)$$

We have introduced shorthand notations, such as $N^{A_1(B_1) \tilde{N}^{A_2)B_2}$, etc., that are obvious generalization of notations previously introduced $N^{(A_1 B_1) \tilde{N}^{A_2 B_2)}$. The harmonics outside the angular brackets are not averaged out.

The corrective terms for the skew spectrum, which is a third-order statistic, depend on linear terms, whereas the trispectrum being a fourth-order statistic, the corrections are quadratic in input harmonics. In addition, it is important to note that the procedure to subtract the Gaussian terms relies on Gaussian simulations. Hence, corrections for the Gaussian subtraction need to be included.

6.4 Corrective terms and subtraction of Gaussian terms

The Gaussian or the disconnected pieces are subtracted from the estimators, as is done in equations (76)–(78). These Gaussian terms too will have to be corrected for partial sky coverage using the technique outlined above. We will outline the procedure for the estimator $\mathcal{K}^{3,1}$; the treatment for the other cases will exactly be the same:

$$\hat{\mathcal{P}}_l^{(A_1^G B_1^G A_2^G, B_2^G)} = \frac{1}{f_{\text{sky}}} \left[\tilde{\mathcal{P}}_l^{(A_1^G B_1^G A_2^G, B_2^G)} - \mathcal{P}_l^{\text{corr}} \right]. \quad (90)$$

The correction term for this Gaussian piece, if written down following the same principle (see equation 80) as the main contribution, takes the following form:

$$\mathcal{P}_l^{\text{corr}} = \frac{1}{f_{\text{sky}}} \left[\mathcal{J}_l^{(A_1 B_1) \langle A_2, B_2 \rangle} + \mathcal{J}_l^{(A_1 A_2) \langle B_1, B_2 \rangle} + \mathcal{J}_l^{(B_1 A_2) \langle A_1, B_2 \rangle} + \mathcal{J}_l^{(A_1 B_1) \langle A_2, B_2 \rangle} + \mathcal{J}_l^{(A_1 A_2) \langle B_1, B_2 \rangle} + \mathcal{J}_l^{(B_1 A_2) \langle A_1, B_2 \rangle} \right] \\ = -\frac{2}{f_{\text{sky}}} \left[\tilde{\mathcal{P}}_l^{(A_1^G B_1^G A_2^G, B_2^G)} \right]. \quad (91)$$

Notice that there are no *free* fields as all contributions are averaged over. The second equality follows from the fact that the correction term by construction is simply twice that of the original Gaussian term. So, the correction simply reverses the signature of the original term. This is consistent with what we found in the derivation of a trispectrum estimator from an Edgeworth expansion in Appendix B (equation B4). The correction to the other contributing term, that is, $\mathcal{R}_l^{\text{corr}}$ can be handled in an analogous manner.

Exactly the same result holds for other estimators.

7 REALISTIC SURVEY STRATEGIES: EXACT ANALYSIS

The discussion so far has ignored the existence of cross-terms. In Appendix A, we have shown why it is not possible to compute the cross-terms that involve computation of $6j$ terms using a map-based method. However, we will see that a method of direct summation can be devised, which will take care of all the contributing terms in a trispectrum. The resulting method does not depend on a specific form of the trispectrum and works with generic models.

We include the full optimization, including the mode–mode coupling introduced by partial sky coverage and inhomogeneous noise, generalizing results from the three-point level (Babich 2005; Smith & Zaldarriaga 2006; Smith et al. 2007, 2009). As before, we find that for the trispectrum, the addition of quadratic terms in addition to linear terms is needed. The analysis presented here is completely generic and does not depend on details of factorizability properties of the trispectrum. For any specific form of the trispectrum, the technique presented here can always provide optimal estimators. Importantly, it makes the technique suitable also for the study of the trispectrum contribution from secondaries and offers the possibility of determining whether any observed connected trispectrum is primordial or not. Generalization to multiple sources of a trispectrum is straightforward, following Smidt et al. (2009).

Trispectra from secondary anisotropies, such as gravitational lensing, are expected to dominate the contribution from primary anisotropies (Cooray & Kesden 2003). The estimator we develop here will be directly applicable to data from various surveys, but the required direct inversion of the covariance matrix in the harmonic domain may not be computationally feasible in near future. Nevertheless an exact analysis may still be beneficial for low-resolution degraded maps where the primary anisotropy dominates. At higher resolution, the exact analysis will reduce to the one discussed in previous sections. In addition, it may be possible at least to certain resolution to bypass the exact inverse variance weighting by introducing a conjugate gradient technique.

The general theory for optimal estimation from data was developed by Babich (2005) for the analysis of the bispectrum and was later implemented by Smith & Zaldarriaga (2006). For arbitrary sky coverage and inhomogeneous noise, the estimator will be of fourth order in input harmonics and involves matched filtering to maximize the response of the estimator when the estimated trispectrum matches theoretical expectation. We present results for both one-point cumulant and two-point cumulant correlators or power spectra associated with trispectra. The estimators presented here, $E_l^{(3,1)}$ and $E_l^{(2,2)}$, are generalizations of the estimators $C_l^{(3,1)}$ and $C_l^{(2,2)}$, and $\mathcal{K}_l^{(3,1)}$ and $\mathcal{K}_l^{(2,2)}$ presented in previous sections.

7.1 One-point estimators

We will use inverse variance weighting harmonics recovered from the sky. The inverse covariance matrix, expressed in the harmonics domain, $C_{lm,l'm'}^{-1}$, is used to filter out modes recovered directly from sky is a_{lm} , and are denoted by \tilde{a}_{lm} . We use these harmonics to construct optimal estimators. For all-sky coverage and homogeneous noise, we can recover $A_{lm} = \frac{\tilde{a}_{lm}}{C_l}$, with the values of C_l including signal and noise. We start by keeping in mind that the trispectrum can be expressed in terms of the harmonic transforms a_{lm} as follows:

$$T_{l_c l_d}^{l_a l_b}(L) = (2L+1) \sum_{m_i} \sum_M (-1)^M \begin{pmatrix} l_a & l_b & L \\ m_a & m_b & M \end{pmatrix} \begin{pmatrix} l_c & l_d & L \\ m_c & m_d & -M \end{pmatrix} a_{l_a m_a} \dots a_{l_d m_d} \quad (i \in a, b, c, d). \quad (92)$$

Based on this expression, we can devise a one-point estimator. In our following discussion, the relevant harmonics can be based on partial sky coverage:

$$Q^{(4)}[a] = \frac{1}{4!} \sum_{LM} (-1)^M \sum_{l_i m_i} T_{l_3 l_4}^{l_1 l_2}(L) \begin{pmatrix} l_a & l_b & L \\ m_a & m_b & M \end{pmatrix} \begin{pmatrix} l_c & l_d & L \\ m_c & m_d & -M \end{pmatrix} a_{l_1 m_1} \dots a_{l_4 m_4}. \quad (93)$$

We will also need the first-order and second-order derivatives with respect to the input harmonics. The linear terms are proportional to the first derivatives and the quadratic terms are proportional to second derivatives of the function $Q[a]$, which is quartic in input harmonics:

$$\partial_{lm} Q^{(4)}[a] = \frac{1}{3!} \sum_{LM} (-1)^M \sum_{l_i m_i} T_{l_c l_d}^{l_a l_b}(L) \begin{pmatrix} l & l_a & L \\ m & m_a & M \end{pmatrix} \begin{pmatrix} l_b & l_c & L \\ m_b & m_c & -M \end{pmatrix} a_{l_a m_b} a_{l_a m_b} a_{l_c m_c}. \quad (94)$$

The first-order derivative term $\partial_{lm} Q^{(4)}[a]$ is cubic in input maps and the second-order derivative is quadratic in input maps (harmonics). However, unlike the estimator itself, $Q^{(4)}[a]$, which is simply a number, these objects represent maps constructed from harmonics of the observed maps:

$$\partial_{lm} \partial_{l'm'} Q^{(4)}[a] = \frac{1}{2!} \sum_{LM} (-1)^M \sum_{l_i m_i} T_{l_c l_d}^{l_a l_b}(L) \begin{pmatrix} l & l_a & L \\ m & m_a & M \end{pmatrix} \begin{pmatrix} l' & l_b & L \\ m' & m_b & -M \end{pmatrix} a_{l_a m_a} a_{l_b m_b}. \quad (95)$$

The optimal estimator for the one-point cumulant can now be written as follows. This is optimal in the presence of partial sky coverage and most general inhomogeneous noise:

$$E^{(4)}[a] = \frac{1}{N} \left\{ Q^{(4)}[C^{-1}a] + \langle [C^{-1}a]_{lm} [C^{-1}a]_{l'm'} \rangle \langle \partial_{lm} \partial_{l'm'} Q^{(4)}[C^{-1}a] \rangle + \text{cyclic permutation} \right. \\ \left. - [C^{-1}a]_{lm} [C^{-1}a]_{l'm'} \langle \partial_{lm} \partial_{l'm'} Q^{(4)}[C^{-1}a] \rangle + \text{cyclic permutation} \right\}. \quad (96)$$

The first term originates from the subtraction of the Gaussian or the disconnected terms and the second term originates from a lack of spherical symmetry. Cyclic permutation of the first term results in two more terms, whereas that of the third term gives another five terms. The normalization is defined in equation (B5).

The estimator can be cast into a simpler form. To do this, we define a function $G^{(4)}[a^G]$ which takes Gaussian harmonics as its input:

$$G^{(4)}[a^G] = \frac{1}{4!} \sum_{LM} (-1)^M \sum_{l_i m_i} T_{l_3 l_4}^{l_1 l_2}(L) \begin{pmatrix} l_a & l_b & L \\ m_a & m_b & M \end{pmatrix} \begin{pmatrix} l_c & l_d & L \\ m_c & m_d & -M \end{pmatrix} a_{l_1 m_1}^G \dots a_{l_4 m_4}^G. \quad (97)$$

The derivatives of $\partial_{lm} \partial_{l'm'} Q_G^{(4)}[C^{-1}a^G]$ are defined accordingly in an analogous way. The partial derivatives are taken with respect to the Gaussian harmonics. We can eventually rewrite equation (96) as

$$T^{(4)}[C^{-1}a] = \frac{1}{N} \left\{ Q^{(4)}[C^{-1}a] - [C^{-1}a]_{lm} [C^{-1}a]_{l'm'} \langle \partial_{lm} \partial_{l'm'} Q^{(4)}[C^{-1}a] \rangle + \text{cyclic permutation} \right\}; \quad (98)$$

$$G^{(4)}[C^{-1}a^G] = \frac{1}{N} \left\{ Q^{(4)}[C^{-1}a^G] - [C^{-1}a^G]_{lm} [C^{-1}a^G]_{l'm'} \langle \partial_{lm} \partial_{l'm'} Q^{(4)}[C^{-1}a^G] \rangle + \text{cyclic permutation} \right\}; \quad (99)$$

$$Q^{(4)}[C^{-1}a] = T^{(4)}[C^{-1}a] - \langle G^{(4)}[C^{-1}a^G] \rangle. \quad (100)$$

It can be shown that $\langle G^{(4)}[C^{-1}a^G] \rangle = -\sum_{lm,l'm'} \langle [C^{-1}a^G]_{lm} [C^{-1}a^G]_{l'm'} \rangle \langle \partial_{lm} \partial_{l'm'} Q^{(4)}[C^{-1}a^G] \rangle$ and we recover the previous form for the estimator (equation 96). The expression for the Fisher matrix, a single number in this particular case, can be computed using the expression $F^{(4)} = \langle [Q^{(4)}]^2 \rangle - \langle Q^{(4)} \rangle^2$, which takes the following form:

$$F^{(4)} = \frac{1}{4!} \frac{1}{N^2} \sum_{LM} \sum_{L'M'} \sum_{(alllm)} \sum_{(alll'm')} (-1)^{M+M'} T_{l_a l_b}^{l_a l_b}(L) T_{l_c l_d}^{l_c l_d}(L) \begin{pmatrix} l_a & l_b & L \\ m_a & m_b & M \end{pmatrix} \begin{pmatrix} l_c & l_d & L \\ m_c & m_d & -M \end{pmatrix} \\ \times \begin{pmatrix} l'_a & l'_b & L' \\ m'_a & m'_b & M' \end{pmatrix} \begin{pmatrix} l'_c & l'_d & L' \\ m'_c & m'_d & -M' \end{pmatrix} \left[C_{l_a m_a, l'_a m'_a}^{-1} \cdots C_{l_d m_d, l'_d m'_d}^{-1} + C_{l_a m_a, l_b m_b}^{-1} C_{l_c m_c, l'_c m'_c}^{-1} C_{l_d m_d, l'_d m'_d}^{-1} \right]. \quad (101)$$

There are two different types of terms. The first type represents the terms without self-coupling. The second type involves self-coupling as represented by $C_{l_a m_a, l_b m_b}^{-1}$ as well as cross-couplings that are represented by inverse covariance matrices of type $C_{l_c m_c, l'_c m'_c}^{-1}$. These terms originate due to the correction from lack of spherical symmetry and will vanish if symmetry is restored.

The ensemble average of this one-point estimator will be a linear combination of parameters f_{NL}^2 and g_{NL} . Estimators constructed at the level of three-point cumulants (Smith & Zaldarriaga 2006; Munshi & Heavens 2010) can be used jointly with this estimator to put independent constraints separately on f_{NL} and g_{NL} . As discussed before, while a one-point estimator has the advantage of higher S/N, such estimators are not immune to contributions from an unknown component, which may not have cosmological origin, such as inadequate foreground separation. The study of these power spectra associated with bispectra or trispectra can be useful in this direction. Note that these direct estimators are computationally expensive due to the inversion and multiplication of large matrices, but can be implemented in low-resolution studies, where primordial signals may be less contaminated by foreground contributions or secondaries.

7.2 Two-point estimators: power spectra associated with trispectra

Generalizing the above expressions for the case of the power spectrum associated with trispectra, we recover the two power spectra we have discussed in previous sections. The information contained in these power spectra is optimal and when summed over L , we can recover the results of one-point estimators:

$$Q_L^{(2,2)}[a] = \frac{1}{4!} \sum_M (-1)^M \sum_{l_i m_i} T_{l_a l_b}^{l_a l_b}(L) \begin{pmatrix} l_a & l_b & L \\ m_a & m_b & M \end{pmatrix} \begin{pmatrix} l_c & l_d & L \\ m_c & m_d & -M \end{pmatrix} a_{l_a m_a} \cdots a_{l_d m_d}. \quad (102)$$

From this definition it is clear that by including the sum over the diagonal of the quadrangle representing the trispectrum, we will recover the one-point estimator $Q^{(4)}$. This is related to the fact that the estimator $Q^{(2,2)}$ probes modes of the trispectrum, keeping the diagonal fixed. The derivatives at first order and second order are as series of maps (for each L) constructed from the harmonics of the observed sky. These are used in the construction of correction terms:

$$\partial_{lm} \partial_{l'm'} Q_L^{(2,2)}[a] = \frac{1}{3!} \sum_T (-1)^M \sum_{l_i m_i} T_{l_a l_b}^{l_a l_b}(L) \begin{pmatrix} l & l_a & L \\ m & m_b & M \end{pmatrix} \begin{pmatrix} l' & l_b & L \\ m' & m_b & -M \end{pmatrix} a_{l_a m_a} a_{l_b m_b}. \quad (103)$$

We can construct the other estimator in a similar manner. To start with, we define the function $Q_L^{(3,1)}[a]$ and construct its first and second derivatives. These are eventually used for construction of the estimator $E_L^{(3,1)}[a]$. As we have seen, both these estimators can be collapsed to a one-point estimator $Q^{(4)}[a]$. As before, the variable a here denotes input harmonics a_{lm} recovered from the noisy-observed sky:

$$Q_L^{(3,1)}[a] = \frac{1}{3!} \sum_M \sum_{ST} (-1)^T a_{LM} \sum_{l_i m_i} T_{l_c l_d}^{L l_b}(T) \begin{pmatrix} L & l_b & S \\ M & m_b & T \end{pmatrix} \begin{pmatrix} l_c & l_d & S \\ m_c & m_d & -T \end{pmatrix} a_{l_b m_b} \cdots a_{l_d m_d}. \quad (104)$$

The derivative term will have two contributing terms corresponding to the derivative with respect to the free index $\{LM\}$ and the terms where indices are summed over, for example, $\{lm\}$, which is very similar to the results for the bispectrum analysis with the estimator $Q_L^{(2,1)}[a]$. One major difference that needs to be taken into account is the subtraction of the Gaussian contribution:

$$\partial_{l'm'} \partial_{LM} Q_L^{(3,1)}[a] = \frac{1}{6} \delta_{lL} \sum_{ST} \sum_{l_i m_i} T_{l_3 l_4}^{L l_2}(T) \begin{pmatrix} l & l_c & S \\ m & m_c & T \end{pmatrix} \begin{pmatrix} l' & l_d & S \\ m' & m_d & -T \end{pmatrix} a_{l_c m_c} a_{l_d m_d}; \quad (105)$$

$$\partial_{lm} \partial_{l'm'} Q_L^{(3,1)}[a] = \frac{1}{6} \sum_M \sum_{l_i m_i} a_{LM} \sum_T T_{l_3 l_4}^{L l_2}(T) \begin{pmatrix} L & l & S \\ M & m & T \end{pmatrix} \begin{pmatrix} l' & l_d & S \\ m' & m_d & -T \end{pmatrix} a_{l_d m_d}. \quad (106)$$

Notice that numerical pre-factors are not important as they will get cancelled when we take into account the normalizing factor. Using these derivatives, we can construct the estimators $E_L^{(3,1)}$ and $E_L^{(2,2)}$:

$$E_L^{(3,1)} = \frac{1}{N} \left\{ Q_L^{(3,1)}[C^{-1}a] + \langle [C^{-1}a]_{lm} [C^{-1}a]_{l'm'} \rangle \left\langle \partial_{lm} \partial_{l'm'} Q_L^{(3,1)}[C^{-1}a] \right\rangle - [C^{-1}a]_{lm} [C^{-1}a]_{l'm'} \left\langle \partial_{lm} \partial_{l'm'} Q_L^{(3,1)}[C^{-1}a] \right\rangle \right\}; \quad (107)$$

$$E_L^{(2,2)} = \frac{1}{N} \left\{ Q_L^{(2,2)}[C^{-1}a] + \langle [C^{-1}a]_{lm} [C^{-1}a]_{l'm'} \rangle \left\langle \partial_{lm} \partial_{l'm'} Q_L^{(2,2)}[C^{-1}a] \right\rangle - [C^{-1}a]_{lm} [C^{-1}a]_{l'm'} \left\langle \partial_{lm} \partial_{l'm'} Q_L^{(2,2)}[C^{-1}a] \right\rangle \right\}. \quad (108)$$

These expressions can also be written in a compact form if we define $G_L^{(2,2)}[a^G]$ and its derivative. The inputs to the function $G_L^{(2,2)}[a^G]$ are the Gaussian harmonics that are used for MC calculations:

$$T_L^{(3,1)}[C^{-1}a] = \frac{1}{N} \left\{ Q_{L'}^{(3,1)}[C^{-1}a] - [C^{-1}a]_{lm} [C^{-1}a]_{l'm'} \langle \partial_{lm} \partial_{l'm'} Q_{L'}^{(3,1)}[C^{-1}a] \rangle \right\}; \quad (109)$$

$$G_L^{(3,1)}[C^{-1}a] = \frac{1}{N} \left\{ Q_{L'}^{(3,1)}[C^{-1}a^G] - [C^{-1}a^G]_{lm} [C^{-1}a^G]_{l'm'} \langle \partial_{lm} \partial_{l'm'} Q_{L'}^{(3,1)}[C^{-1}a^G] \rangle \right\}; \quad (110)$$

$$E_L^{(3,1)}[C^{-1}a] = T_L^{(3,1)}[C^{-1}a] - \langle G_L^{(3,1)}[C^{-1}a^G] \rangle; \quad (111)$$

where summation over L' is implied in both set of equations. A similar set of expressions can be devised for the other two-point estimator, namely $E_L^{(2,2)}$. The normalization constants are related to the Fisher matrix elements for the spherically symmetric case $\sum_{LL'} F_{LL'} = \frac{1}{N}$, which can be expressed in terms of the target trispectra $T_{l_3 l_4}^{l_1 l_2}(L)$ and inverse covariance matrices C^{-1} used for the construction of these estimators. The Fisher matrix encodes the information about the covariance structure of the estimators, which for a generic estimator, E_L , is defined as $F_{LL'} = \langle E_L E_{L'} \rangle - \langle E_L \rangle \langle E_{L'} \rangle$. The Fisher matrix for the estimator $E_L^{(3,1)}$, that is, $F_{LL'}^{(3,1)}$ can be expressed as

$$\begin{aligned} F_{LL'}^{(3,1)} &= \left(\frac{1}{4!} \right)^2 \frac{1}{N^2} \sum_{ST, S'T'} \sum_{(alllm, l'm')} (-1)^{M+M'} \left[T_{l_c l_d}^{l_a l_b}(L) \right] \left[T_{l'_c l'_d}^{l'_a l'_b}(L') \right] \\ &\times \begin{pmatrix} l_a & l_b & S \\ m_a & m_b & T \end{pmatrix} \begin{pmatrix} L & l_d & S \\ M & m_d & -T \end{pmatrix} \begin{pmatrix} l'_a & l'_b & S' \\ m'_a & m'_b & T' \end{pmatrix} \begin{pmatrix} L' & l'_d & S' \\ M' & m'_d & -T' \end{pmatrix} \\ &\times \left\{ 6C_{LM, L'M'}^{-1} C_{l_a m_a, l'_a m'_a}^{-1} C_{l_b m_b, l'_b m'_b}^{-1} C_{l_c m_c, l'_c m'_c}^{-1} + 18C_{LM, L'M'}^{-1} C_{l_a m_a, L'M'}^{-1} C_{l_b m_b, l'_b m'_b}^{-1} C_{l_c m_c, l'_c m'_c}^{-1} \right\}. \end{aligned} \quad (112)$$

We have not included the terms that originate from the quadratic corrections, which can be derived following the same logic outlined for the one-point estimator. Similarly, for the other estimator $E_L^{(2,2)}$, the Fisher matrix $F_{LL'}^{(2,2)}$ can be written as a function of the associated trispectrum and the covariance matrix of various modes. For further simplification of these expressions, we need to make simplifying assumptions for a specific type of trispectra (see Munshi & Heavens 2010 for more details for such simplifications in the bispectrum):

$$\begin{aligned} F_{LL'}^{(2,2)} &= \left(\frac{1}{4!} \right) \frac{1}{N^2} \sum_M \sum_{M'} \sum_{(alllm)} \sum_{(alll'm')} (-1)^{M+M'} T_{l_c l_d}^{l_a l_b}(L) T_{l'_c l'_d}^{l'_a l'_b}(L') \begin{pmatrix} l_a & l_b & L \\ m_a & m_b & M \end{pmatrix} \begin{pmatrix} l_c & l_d & L \\ m_c & m_d & -M \end{pmatrix} \\ &\times \begin{pmatrix} l'_a & l'_b & L' \\ m'_a & m'_b & M' \end{pmatrix} \begin{pmatrix} l'_c & l'_d & L' \\ m'_c & m'_d & -M' \end{pmatrix} C_{l_a m_a, l'_a m'_a}^{-1} \dots C_{l_d m_d, l'_d m'_d}^{-1}. \end{aligned} \quad (113)$$

Knowledge of sky coverage and the noise characteristics resulting from a specific scanning strategy, etc., is needed for modelling of $C_{l_d m_d, l'_d m'_d}^{-1}$. We will discuss the impact of inaccurate modelling of the covariance matrix in the next section. The direct summation we have used for the construction of the Fisher matrix may not be feasible except for low-resolution studies. However, a hybrid method may be employed to combine the estimates from low-resolution maps by using exactly the same method as used with estimates from higher resolution using other faster but optimal techniques described in the previous section. In certain situations when the data are noise dominated, further approximation can be made to simplify the implementation. A more detailed discussion will be presented elsewhere.

On a different note, it is possible to form linear combination of $D'_L = \sum_{L'} S_{L'}^{-1} E_{L'}$; here specific choices for M will result in different sets of estimators D'_L , for example, $S = F^{1/2}$ can lead to estimators with an unit error covariance.

7.3 Approximation to exact C^{-1} weighting and non-optimal weighting

If the covariance matrix is not accurately known due to the lack of exact beam or noise characteristics, or due to limitations on computer resources, it can be approximated. An approximation R of C^{-1} then acts as a regularization method. The corresponding generic estimator can then be expressed as

$$\hat{E}_L^Z[a] = \frac{1}{N} \left\{ Q_{L'}^Z[Ra] - [Ra]_{lm} [Ra]_{l'm'} \langle \partial_{lm} \partial_{l'm'} Q_{L'}^Z[Ra] \rangle \right\}; \quad Z \in \{(2, 2), (3, 1)\}. \quad (114)$$

As before we have assumed sums over repeated indices and $\langle \cdot \rangle$ denotes MC averages. As evident from the notations, the estimator above can be of type $E_L^{(3,1)}$ or $E_L^{(2,2)}$. For the collapsed case, $E_L^{(4)}$ can also be handled in a very similar manner:

$$\hat{E}[a] = \frac{1}{N} \left\{ Q[Ra] - [Ra]_{lm} [Ra]_{l'm'} \langle \partial_{lm} \partial_{l'm'} Q[Ra] \rangle \right\}. \quad (115)$$

We will drop the superscript Z for simplicity but any conclusion drawn below will be valid for both specific cases, that is, $Z \in \{(2, 2), (3, 1)\}$. The normalization constant is defined in terms of the associated Fisher matrix F^R ; $\sum_{LL'} F_{LL'}^R = \frac{1}{N_R}$. Here, the superscript R denotes Fisher matrix associated with an estimator that uses arbitrary regularization R instead of inverse covariance–variance weighting. The construction of $F_{LL'}^R$ is equivalent to the calculation presented for the case of $R = C^{-1}$. For a one-point estimator, we can similarly write $E^{(4)} = \sum_L E_L^{(3,1)} = \sum_L E_L^{(2,2)}$. The optimal weighting can be replaced by arbitrary weighting. As a special case, we can also use no weighting

at all $R = I$. Although the estimator remains unbiased, the scatter, however, increases as the estimator is no longer optimal. Use of arbitrary weights makes the estimator equivalent to a PCL estimator.

7.4 Joint estimation of multiple trispectra

It is also of interest to estimate several trispectra jointly. In such scenarios, it is indeed important to construct a joint Fisher matrix. This will be interesting for computing cross-contamination between estimates of primary trispectra and the ones generated by secondaries (e.g. lensing). For two generic estimators E^X and E^Y , X and Y correspond to different trispectra of type X and Y , which could also be, for example, primordial trispectra from various inflationary scenarios; it is possible of course to do a joint estimation. The off-diagonal blocks of the Fisher matrix will correspond to cross-talks between various types of trispectra. Indeed, Principal Component Analysis or generalized eigenmode analysis can be useful in finding how many independent components of such trispectra can be estimated from the data.

The cross-terms in the Fisher matrix elements will be of the following type:

$$F_{LL'}^{XY} = \left(\frac{1}{4!}\right)^2 \frac{1}{N^X N^Y} \sum_{ST, S'T'} \sum_{(all m, l' m')} (-1)^M (-1)^{M'} \left[T_{l_c l_c}^{l_a l_b}(L) \right]^X \left[T_{l_c' l_c'}^{l_a' l_b'}(L') \right]^Y \\ \times \begin{pmatrix} l_a & l_b & S \\ m_a & m_b & T \end{pmatrix} \begin{pmatrix} L & l_d & S \\ M & m_d & -T \end{pmatrix} \begin{pmatrix} l'_a & l'_b & S' \\ m'_a & m'_b & T' \end{pmatrix} \begin{pmatrix} L' & l'_d & S' \\ M' & m'_d & -T' \end{pmatrix} \\ \times \left\{ 6C_{LM, L'M'}^{-1} C_{l_a m_a, l'_a m'_a}^{-1} C_{l_b m_b, l'_b m'_b}^{-1} C_{l_c m_c, l'_c m'_c}^{-1} + 18C_{LM, l'_a m'_a}^{-1} C_{l_a m_a, L'M'}^{-1} C_{l_b m_b, l'_b m'_b}^{-1} C_{l_c m_c, l'_c m'_c}^{-1} \right\}. \quad (116)$$

The normalization constants N^X and N^Y correspond to two different types of trispectra.

The expression displayed above is valid only for $E^{(3,1)}$; exactly similar results hold for the other estimator $E^{(3,1)}$. For $X = Y$, we recover the results presented in the previous section for independent estimates. As before, we recover the usual result for a one-point estimator for Q^4 from the Fisher matrix of $Q_L^{(3,1)}$ or $Q_L^{(2,2)}$, with the corresponding estimator modified accordingly.

A joint estimation can provide clues to cross-contamination from different sources of trispectra. It also provides information about the level of degeneracy involved in such estimates.

8 CONCLUSIONS

In the near future, the all-sky *Planck* satellite will complete mapping the CMB sky in unprecedented detail, covering a huge frequency range. The cosmological community will have the opportunity to use the resulting data to constrain available theoretical models. While the power spectrum provides the bulk of the information, going beyond this level will lift degeneracies amongst various early universe scenarios, which otherwise have near-identical power spectra. The higher order spectra are the harmonic transforms of multipoint correlation functions, which contain information, which can be difficult to extract using conventional techniques. This is related to their complicated response to inhomogeneous noise and sky coverage. A practical advance is to form collapsed two-point statistics, constructed from higher order correlations, which can be extracted using conventional power-spectrum estimation methods.

We have specifically studied and developed three different types of estimators, which can be employed to analyse these power spectra associated with higher order statistics. The MASTER-based approach (Hivon et al. 2002) is typically employed to estimate PCLs from the masked sky in the presence of noise (see also Efstathiou 2004, 2006). These are unbiased estimators but the associated variances and scatter can be estimated analytically with very few simplifying assumptions. We extend these estimators to study higher order correlation functions. We develop estimators for $C_l^{(2,1)}$ for the skew spectrum (three-point) as well as for $C_l^{(3,1)}$ and $C_l^{(2,2)}$, which are power spectra related to the trispectrum or the kurt spectrum (four-point). The removal of the Gaussian contribution is achieved by applying the same estimators to a set of Gaussian simulations with identical power spectra and subtracting.

As a next step, we generalized the estimators employed by Yadav, Komatsu & Wandelt (2007), Yadav & Wandelt (2008), Yadav et al. (2008) and others to study the kurt spectrum. These methods are computationally expensive and can be implemented using a MC pipeline, which can generate three-dimensional maps from the cut-sky harmonics using radial integrations of a target theoretical model. The MC generation of three-dimensional maps is the most computationally expensive part and dominates the calculation. The technique nevertheless has been used extensively, as it remains highly parallelizable and is optimal in the presence of homogeneous noise and near all-sky coverage. The corrective terms involve quadratic terms for lack of spherical symmetry due to inhomogeneous noise and partial sky coverage. These terms can be computed using a MC chain. We also showed that the radial integral involved at the three-point analysis needs to be extended to a double integral for the trispectrum. The speed of this analysis depends on how fast we can generate non-Gaussian maps. It is also possible to use the same formalism to study cross-contamination from other sources, such as point sources or other secondaries, while also determining primordial non-Gaussianity. The analysis also allows us to compute the overlap or degeneracy among various theoretical models for primordial non-Gaussianity. We point out various advantages and pitfalls in using this approach in great detail. We discuss various schemes to develop optimum estimators and present detailed derivations to show how there are underlying connections in various approaches.

Finally, we presented the analysis for the case of estimators, which are completely optimal even in the presence of inhomogeneous noise and arbitrary sky coverage (Smith & Zaldarriaga 2006). Extending previous work by Munshi & Heavens (2010), which concentrated only on the skew spectrum, we showed how to generalize to the trispectrum. This involves finding a fast method to construct and invert

the covariance matrix $C_{lm'l'm'}$ in multipole space. In most practical circumstances, it is possible only to find an approximation to the exact covariance matrix and to cover this we present analysis for an approximate matrix, which can be used instead of C^{-1} . This makes the method marginally suboptimal, but it remains unbiased. The four-point correlation function also takes contributions which are purely Gaussian in nature. The subtraction of these contributions is again simplified by the use of Gaussian MC maps with the same power spectrum. A Fisher analysis was presented for the construction of the error covariance matrix, allowing joint estimation of trispectrum contributions from various sources, primaries or secondaries. Such a joint estimation gives us fundamental limits on how many sources of non-Gaussianity can be jointly estimated from a specific experimental setup. A more detailed Karhunen–Loève eigenmode analysis will be presented elsewhere. The detection of non-primordial effects, such as weak lensing of the CMB, the kSZ effect, the Ostriker–Vishniac effect and the tSZ effect, can provide valuable additional cosmological information (Riquelme & Spergel 2007). The detection of CMB lensing at the level of the bispectrum needs external data sets, which trace large-scale structures, but the trispectrum offers an internal detection, albeit with reduced S/N, providing a valuable consistency check.

At the level of the bispectrum, primordial non-Gaussianity for many models can be described by a single parameter f_{NL} . The two degenerate kurt spectra (power spectra related to trispectra) we have studied at the four-point level require, typically, two parameters, such as f_{NL} and g_{NL} . Use of the two power spectra will enable us to put separate constraints on f_{NL} and g_{NL} without using information from lower order analysis of bispectra, but they can all be used in combination. Clearly, at even higher order, more parameters will be needed to describe various models (f_{NL} , g_{NL} , h_{NL} , ...) all of which will be essential in describing degenerate sets of power spectra associated with multispectra at a specific level. Note that we should keep in mind that higher order spectra will be progressively more dominated by noise and may not provide useful information beyond a certain point.

The power of the estimators we have constructed largely depends on finding a technique to simulate non-Gaussian maps with a specified bispectrum and trispectrum. We have discussed the possibility of using our technique to generate all-sky CMB maps with specified lower order spectra, that is, power spectra, bispectra and trispectra. These will generalize previous results by Smith & Zaldarriaga (2006), which can guarantee a specific form at bispectrum level.

While we have primarily focused on CMB studies, our estimators can also be useful in other areas, for example, studies involving 21-cm studies, near all-sky redshift surveys and weak-lensing surveys. The estimators described here can be useful for testing theories for primordial and/or gravity-induced secondary trispectra using such diverse data sets. As already pointed out, in the near future, all-sky CMB experiments, such as *Planck*, can provide maps covering a huge frequency range and near-all sky coverage. The estimators described here can play a valuable role in analysing such maps.

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APPENDIX A: SYMMETRY CONSIDERATIONS AND OPTIMIZED TRISPECTRUM ESTIMATOR

In the text of this paper, we have considered an approximation to replace the trispectrum with its reduced counterpart. In this appendix, we point out how some of the additional terms can also be incorporated using a map-based technique. We also write down the expressions for the terms that can only be evaluated using a direct summation over harmonic modes, which leads to development of more generic estimators. The results will be demonstrated using the estimator $\mathcal{K}_l^{(2,2)}$, but very similar steps will lead to equivalent results for the other estimator $\mathcal{K}_l^{(3,1)}$.

The trispectrum $T_{l_3 l_4}^{l_1 l_2}(l)$ can be expressed in terms of the reduced trispectrum $P_{l_3 l_4}^{l_1 l_2}(l)$. The following expression was introduced by Hu (2001) and encodes all possible inherent symmetries:

$$T_{l_3 l_4}^{l_1 l_2}(l) = P_{l_3 l_4}^{l_1 l_2}(l) + (2l+1) \left[\sum (-1)^{l_2+l_3} \begin{Bmatrix} l_1 & l_2 & l \\ l_4 & l_3 & l' \end{Bmatrix} P_{l_2 l_4}^{l_1 l_3}(l') + \sum (-1)^{L+L'} \begin{Bmatrix} l_1 & l_2 & l \\ l_3 & l_4 & l' \end{Bmatrix} P_{l_3 l_2}^{l_1 l_4}(l') \right]. \quad (\text{A1})$$

The matrices in curly brackets represent $6j$ symbols and can be defined using $3j$ symbols (see equation D1). The entities $P_{l_3 l_4}^{l_1 l_2}(l)$ can be further decomposed in terms of the *reduced* trispectrum $\tau_{l_3 l_4}^{l_1 l_2}(l)$, which was introduced in the main text (equation 39):

$$P_{l_3 l_4}^{l_1 l_2}(l) = \tau_{l_3 l_4}^{l_1 l_2}(l) + (-1)^{\Sigma_U} \tau_{l_3 l_4}^{l_2 l_1}(l) + (-1)^{\Sigma_L} \tau_{l_4 l_3}^{l_1 l_2}(l) + (-1)^{\Sigma_L + \Sigma_U} \tau_{l_4 l_3}^{l_2 l_1}(l). \quad (\text{A2})$$

In our discussion, in the text of this paper, we have considered the near-optimal estimators, where the estimators were constructed from $\tau_{l_3 l_4}^{l_1 l_2}(l)$. However, we will show here that all additional contributions, such as $(-1)^{\Sigma_U} \tau_{l_3 l_4}^{l_2 l_1}(l)$, $(-1)^{\Sigma_L} \tau_{l_4 l_3}^{l_1 l_2}(l)$ and $(-1)^{\Sigma_U + \Sigma_L} \tau_{l_4 l_3}^{l_2 l_1}(l)$, that appear in the definition of $P_{l_3 l_4}^{l_1 l_2}(l)$ make identical contributions (we have introduced the notations $\Sigma_U = l_1 + l_2 + l$ and $\Sigma_L = l_3 + l_4 + l$). This implies that we do not need to construct estimators for each of such individual terms. We also show that the map-based methods that are usually employed in the estimation of the skew spectrum *cannot* be extended directly to the case of power spectra associated with a trispectrum (or kurt spectrum) to include other terms that involve $6j$ symbols.

A1 The fundamental term: $\tau_{l_3 l_4}^{l_1 l_2}(l)$

The power spectrum that we will construct from the fundamental term will involve line-of-sight integrations:

$$C_l^{AB,AB} = \int r_1^2 dr_1 \int r_2^2 dr_2 C_l^{AB,AB}(r_1, r_2); \quad C_l^{AB,AB}(r_1, r_2) = \frac{1}{2l+1} \sum_m F_l(r_1, r_2) [A(r_1)B(r_1)] [A(r_2)B(r_2)]^*. \quad (\text{A3})$$

To derive the estimators, we can start from the definition of $A(r)$ and $B(r)$ (see equation 43 for the definitions) and construct the harmonics of the product field $[A(r_1)B(r_1)]$. Both fields are evaluated at the same radial distance r_1 :

$$[A(r_1)B(r_1)]_{lm} = \sum_{l_1 m_1} \sum_{l_2 m_2} \frac{\alpha_{l_1}(r_1)}{C_{l_1}} \frac{\beta_{l_2}(r_1)}{C_{l_2}} a_{l_1 m_1} a_{l_2 m_2} \int d\hat{\Omega} Y_{l_1 m_1}(\hat{\Omega}) Y_{l_2 m_2}(\hat{\Omega}) Y_{lm}^*(\hat{\Omega}). \quad (\text{A4})$$

We use the relationship $Y_{lm}^* = (-1)^m Y_{l-m}$, which introduces a factor of $(-1)^m$:

$$[A(r_1)B(r_1)]_{lm} = \sum_{l_1 m_1} \sum_{l_2 m_2} \frac{\alpha_{l_1}(r_1)}{C_{l_1}} \frac{\beta_{l_2}(r_1)}{C_{l_2}} a_{l_1 m_1} a_{l_2 m_2} (-1)^m h_{l_1 l_2 l} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}. \quad (\text{A5})$$

Next we construct the same harmonics, again using the expression for the Gaunt integral (equation C5) of the same product field at a different radial distance r_2 :

$$[A(r_2)B(r_2)]_{lm}^* = \sum_{l_3 m_3} \sum_{l_4 m_4} \frac{\alpha_{l_3}(r_2)}{C_{l_3}} \frac{\beta_{l_4}(r_2)}{C_{l_4}} (-1)^{2(m_3+m_4)} a_{l_3 -m_3} a_{l_4 -m_4} h_{l_3 l_4 l} \begin{pmatrix} l_3 & l_4 & l \\ -m_3 & -m_4 & m \end{pmatrix}. \quad (\text{A6})$$

In this expression, the first set of $(-1)^{(m_3+m_4)}$ results from changing $Y_{l_3 m_3}^*$ and $Y_{l_4 m_4}^*$ to $Y_{l_3 -m_3}$ and $Y_{l_4 -m_4}$, whereas the second set results from changing $a_{l_3 m_3}^*$ to $a_{l_3 -m_3}$ and likewise for the other sets. We use the relations $Y_{lm}^* = (-1)^m Y_{l-m}$ and $a_{lm}^* = (-1)^m a_{l-m}$.

$$C_l^{AB,AB} = \sum_m \sum_{m_i} \sum_{l_i} (-1)^m F_l(r_1, r_2) \frac{\alpha_{l_1}(r_1)}{C_{l_1}} \frac{\beta_{l_2}(r_1)}{C_{l_2}} \frac{\alpha_{l_3}(r_2)}{C_{l_3}} \frac{\beta_{l_4}(r_2)}{C_{l_4}} h_{l_1 l_2 l} h_{l_3 l_4 l} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} \times \begin{pmatrix} l_3 & l_4 & l \\ -m_3 & -m_4 & m \end{pmatrix} \langle a_{l_1 m_1} a_{l_2 m_2} a_{l_3 -m_3} a_{l_4 -m_4} \rangle. \quad (\text{A7})$$

We only have the surviving factor $(-1)^m$ above as $(-1)^{2(m_3+m_4)} = 1$. We will use the definition of the trispectrum $T_{l_3 l_4}^{l_1 l_2}(l)$ next to simplify the above expression (equation 14). Using further the identity in equation (C3), we can finally obtain the following expression:

$$C_l^{AB,AB} = \int r_1^2 dr_1 \int r_2^2 dr_2 C_l^{AB,AB}(r_1, r_2) = \frac{1}{2l+1} \sum_{l_i} \frac{1}{2l+1} \frac{\tau_{l_3 l_4}^{l_1 l_2}(l) T_{l_3 l_4}^{l_1 l_2}(l)}{C_{l_1} C_{l_2} C_{l_3} C_{l_4}}, \quad (\text{A8})$$

where we have the following expression for $\tau_{l_3 l_4}^{l_1 l_2}(l)$:

$$\tau_{l_3 l_4}^{l_1 l_2}(l) = h_{l_1 l_2 l} h_{l_3 l_4 l} \int r_1^2 dr_1 \int r_2^2 dr_2 F_l(r_1, r_2) \alpha_{l_1}(r_1) \beta_{l_2}(r_1) \alpha_{l_3}(r_2) \beta_{l_4}(r_2). \quad (\text{A9})$$

We have considered only the first component of $\tau_{l_3 l_4}^{l_1 l_2}(l)$, but the other component, which corresponds to the correlations of the product fields $BM(\hat{\Omega}, r)$ and $B^3(\hat{\Omega}, r)$, can also be dealt with in an exactly similar manner.

A2 Second term $(-1)^{l_1+l_2+l} \tau_{l_3 l_4}^{l_1 l_2}(l)$

If we start by exchanging the indices l_1 and l_2 in equation (A7), we will get the following expression:

$$C_l^{AB,AB}(r_1, r_2) = \sum_m \sum_{m_i} \sum_{l_i} (-1)^m F_l(r_1, r_2) \frac{\alpha_{l_1}(r_1)}{C_{l_2}} \frac{\beta_{l_2}(r_1)}{C_{l_2}} \frac{\alpha_{l_3}(r_2)}{C_{l_3}} \frac{\beta_{l_4}(r_2)}{C_{l_4}} h_{l_2 l_1 l} h_{l_3 l_4 l} \begin{pmatrix} l_2 & l_1 & l \\ m_1 & m_2 & -m \end{pmatrix} \\ \times \begin{pmatrix} l_3 & l_4 & l \\ -m_3 & -m_4 & m \end{pmatrix} \langle a_{l_1 m_1} a_{l_2 m_2} a_{l_3 -m_3} a_{l_4 -m_4} \rangle. \quad (\text{A10})$$

We will use the identity in equation (C1) that encodes the exchange symmetry of $3j$ symbols. This means we pick up an additional factor of $(-1)^{l_1+l_2+l}$. The rest of the analysis follows an exactly similar way and the resulting expression takes the following form:

$$C_l^{AB,AB} = \int r_1^2 dr_1 \int r_2^2 dr_2 C_l^{AB,AB}(r_1, r_2) = \frac{1}{2l+1} \sum_{l_i} \frac{1}{2l+1} \frac{(-1)^{\Sigma_U} \tau_{l_3 l_4}^{l_2 l_1}(l) T_{l_3 l_4}^{l_1 l_2}(l)}{C_{l_1} C_{l_2} C_{l_3} C_{l_4}}, \quad (\text{A11})$$

where $\tau_{l_3 l_4}^{l_2 l_1}(l)$ is obtained by exchanging l_1 and l_2 .

A3 Third and fourth terms

The other two contributions can be treated in a similar manner. First, if we exchange the indices l_3 and l_4 , then we obtain

$$C_l^{AB,AB} = \int r_1^2 dr_1 \int r_2^2 dr_2 C_l^{AB,AB}(r_1, r_2) = \frac{1}{2l+1} \sum_{l_i} \frac{1}{2l+1} \frac{(-1)^{\Sigma_L} \tau_{l_4 l_3}^{l_1 l_2}(l) T_{l_3 l_4}^{l_1 l_2}(l)}{C_{l_1} C_{l_2} C_{l_3} C_{l_4}}, \quad (\text{A12})$$

and finally by simultaneous exchange of l_1 and l_2 as well as of l_3 and l_4 , we obtain the following expression:

$$C_l^{AB,AB} = \int r_1^2 dr_1 \int r_2^2 dr_2 C_l^{AB,AB}(r_1, r_2) = \frac{1}{2l+1} \sum_{l_i} \frac{1}{2l+1} \frac{(-1)^{\Sigma_U + \Sigma_L} \tau_{l_4 l_3}^{l_2 l_1}(l) T_{l_3 l_4}^{l_1 l_2}(l)}{C_{l_1} C_{l_2} C_{l_3} C_{l_4}}. \quad (\text{A13})$$

A4 Total contribution from the direct term

Adding all these individual contributions, we finally get

$$4C_l^{AB,AB} = \frac{1}{2l+1} \sum_{l_i} \frac{1}{2l+1} \left\{ \tau_{l_3 l_4}^{l_1 l_2}(l) + (-1)^{\Sigma_U} \tau_{l_3 l_4}^{l_2 l_1}(l) + (-1)^{\Sigma_L} \tau_{l_4 l_3}^{l_1 l_2}(l) + (-1)^{\Sigma_L + \Sigma_U} \tau_{l_4 l_3}^{l_2 l_1}(l) \right\} \frac{T_{l_3 l_4}^{l_1 l_2}(l)}{C_{l_1} C_{l_2} C_{l_3} C_{l_4}}; \quad (\text{A14})$$

$$4C_l^{AB,AB} = \frac{1}{2l+1} \sum_{l_i} \frac{1}{2l+1} \frac{P_{l_3 l_4}^{l_1 l_2}(l) T_{l_3 l_4}^{l_1 l_2}(l)}{C_{l_1} C_{l_2} C_{l_3} C_{l_4}}. \quad (\text{A15})$$

The subtraction of Gaussian terms will follow from the same logic. The other contribution to the trispectrum can be handled in a similar way.

The above expression includes the entire trispectrum in $\hat{T}_{l_3 l_4}^{l_1 l_2}(l)$ and only replaces the target trispectrum $T_{l_3 l_4}^{l_1 l_2}(l)$ with $P_{l_3 l_4}^{l_1 l_2}(l)$. The idea of replacing $T_{l_3 l_4}^{l_1 l_2}(l)$ with $P_{l_3 l_4}^{l_1 l_2}(l)$ was initially considered in Hu (2001). The construction presented above shows how to achieve it in analysing real data. The remaining terms can only be incorporated using a direct summation technique, which we consider next.

A5 Contributions from the cross-terms involving $6j$ symbols

So far we have considered only those terms that can directly be constructed from the fundamental term. These terms can be estimated using map-based methods, which are discussed in Section 7. The map-based techniques are computationally less expensive as they only require harmonic transforms. However, in addition to these terms that we have considered above, there are additional terms that contain the $6j$ symbols or the *cross-terms* and are more expensive to implement numerically. However, it is known from previous studies that these cross-terms are subdominant in many practical situations (Hu 2001; Kogo & Komatsu 2006). Nevertheless, these cross-terms can be implemented using direct sums of the harmonic coefficients a_{lm} of the temperature maps. The two cross-terms are constructed from the other two contributions, namely $P_{l_2 l_4}^{l_1 l_3}(l)$ and $P_{l_3 l_2}^{l_1 l_4}(l)$.

If we consider the second term in the above expression (equation A1), then the relevant contribution to the two-to-two power spectrum can be expressed as follows:

$$C_l^{(2,2)}(r_1, r_2) = \sum_{l'} \sum_{l_i} \sum_{m_i} (-1)^{l_2+l_3} h_{l_1 l_3 l'} h_{l_2 l_4 l'} \frac{\alpha_{l_1}(r_1)}{C_{l_1}} \frac{\beta_{l_3}(r_1)}{C_{l_3}} \frac{\alpha_{l_2}(r_2)}{C_{l_2}} \frac{\beta_{l_4}(r_2)}{C_{l_4}} F_{l'}(r_1, r_2) \\ \times \begin{Bmatrix} l_1 & l_2 & l \\ l_4 & l_3 & l' \end{Bmatrix} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & m \end{pmatrix} \begin{pmatrix} l_3 & l_4 & l \\ -m_3 & -m_4 & m \end{pmatrix} a_{l_1 m_1} a_{l_2 m_2} a_{l_3 -m_3} a_{l_4 -m_4}. \quad (\text{A16})$$

The remaining terms that involve internal permutations, such as $\tau_{l_2 l_4}^{l_3 l_1}$, $\tau_{l_4 l_2}^{l_1 l_3}$ or $\tau_{l_4 l_2}^{l_3 l_1}$, can likewise be constructed in an analogous manner by introducing relevant powers of (-1) and rearrangement of indices. The final estimator will have to take into account the integration along the radial directions, that is, variables r_1 and r_2 have to be integrated out, as was the case in, for example, equations (A11) and (A13).

It is possible to construct an estimator which includes the full trispectrum. The estimators that we have constructed in Section 7 include all terms for an arbitrary trispectrum. This is achieved by incorporating direct summation of modes in a way similar to what is outlined above but for generic trispectra. Such an estimator has an added advantage that it can be useful for the estimation of the type of trispectra, which cannot be factorized.

On a different note, we also point out that the cross-terms involving $6j$ symbols do not arise in the context-bispectrum or skew-spectrum estimators, where all-contributing terms can be constructed from a single map-based operation.

APPENDIX B: MATHEMATICAL BASIS FOR AN OPTIMAL ESTIMATOR

In this appendix, we present the basic framework that was used in the construction of the estimators that we have introduced in the main text. The fundamental assumption in the development of these estimators is that of weak non-Gaussianity, which allows us to expand a *generic* non-Gaussian probability distribution function (PDF) in terms of a Gaussian PDF and a series based on the cumulants of the target distribution. If we assume the sky to be Gaussian and is defined through a set of harmonics $A = \{a_{lm}\}$ with covariance matrix $C = AA^T = \langle a_{lm} a_{l'm'}^* \rangle$, the associated Gaussian probability distribution function denoted by $P_G(A)$ can be expressed as

$$P_G(A) = \frac{1}{(2\pi)^{n/2} ||C||^{1/2}} \exp \left[-\frac{1}{2} (AC^{-1}A^T) \right], \quad (B1)$$

where n denotes the total number of modes, $n = \sum_{l_i=2}^{l_{\max}} (2l_i + 1)$, used to represent the CMB sky and $||C||$ is the determinant of the covariance matrix C . Coupling of modes represents deviations from Gaussianity and the resulting PDF is no longer a non-Gaussian one. The fractional change in the PDF δP can be expressed in terms of the lower order moments as

$$\frac{\delta P}{P} = - \left[\sum_{l_i m_i} \langle a_{l_1 m_1} a_{l_2 m_2} a_{l_3 m_3} \rangle \partial_{l_1 m_1} \partial_{l_2 m_2} \partial_{l_3 m_3} + \sum_{l_i m_i} \langle a_{l_1 m_1} a_{l_2 m_2} a_{l_3 m_3} a_{l_4 m_4} \rangle_c \partial_{l_1 m_1} \partial_{l_2 m_2} \partial_{l_3 m_3} \partial_{l_4 m_4} + \dots \right]; \quad \partial_{l_i m_i} \equiv \frac{\partial}{\partial a_{l_i m_i}} \quad (B2)$$

The subscript ‘c’ denotes the connected part of the trispectrum. In construction of the optimum trispectrum estimator, the contribution from the bispectrum or the first term is usually ignored, which allows the equation to be recast in a way that can be useful for writing down a optimal estimator for the trispectrum:

$$P(A) = [1 + \sum_{l_i m_i} \langle a_{l_1 m_1} a_{l_2 m_2} a_{l_3 m_3} a_{l_4 m_4} \rangle_c \left[(C^{-1}a)_{l_1 m_1} (C^{-1}a)_{l_2 m_2} (C^{-1}a)_{l_3 m_3} (C^{-1}a)_{l_4 m_4} \right. \\ \left. - \left\{ (C^{-1})_{l_1 m_1, l_2 m_2} (C^{-1}a)_{l_3 m_3} (C^{-1}a)_{l_4 m_4} + \text{cyclic permutation} \right\} + \left\{ C_{l_1 m_1, l_2 m_2}^{-1} C_{l_3 m_3, l_4 m_4}^{-1} + \text{cyclic permutation} \right\} + \dots \right]; \quad (B3)$$

The first bracket includes quadratic terms. There will be additional five terms that can be constructed by cyclic permutation of the term shown. The second bracket contains terms that are pure numbers; it takes into account another two terms that are cyclic permutations of the term depicted. The first set of terms (a total of six) represents the quadratic corrections due to lack of spherical symmetry and the second set of terms represents the subtraction of disconnected terms or Gaussian contributions. The quadratic correction terms in equation (89) for the one-point estimator correspond to the quadratic terms presented here. The quadratic correction terms listed in equations (80) and (82) for $\mathcal{K}_l^{(3,1)}$, as well as in equations (85) and (87) for $\mathcal{K}_l^{(2,2)}$, for these two-point estimators too trace their origin to the quadratic terms in the above equation.

The optimal estimator is recovered by maximizing the change in PDF with respect to the trispectrum and is similar to derivation of the bispectrum estimator (see Regan, Shellard & Fergusson 2010 for detailed derivation):

$$E[\tilde{a}] = \frac{1}{N} \sum_{l_i m_i} \sum_{LM} (-1)^M T_{l_3 l_4}^{l_1 l_2}(L) \begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & M \end{pmatrix} \begin{pmatrix} l_3 & l_4 & L \\ m_3 & m_4 & -M \end{pmatrix} \\ \times [\tilde{a}_{l_1 m_1} \tilde{a}_{l_2 m_2} \tilde{a}_{l_3 m_3} \tilde{a}_{l_4 m_4} - \{ C_{l_1 m_1, l_2 m_2}^{-1} \tilde{a}_{l_3 m_3} \tilde{a}_{l_4 m_4} + \text{cyclic permutation} \} + \{ C_{l_1 m_1, l_2 m_2}^{-1} C_{l_3 m_3, l_4 m_4}^{-1} + \text{cyclic permutation} \}]; \\ \tilde{a}_{lm} = C_{lm, l'm'}^{-1} a_{l'm'}. \quad (B4)$$

The normalization constant N and the normalization matrix $N_{LL'}$ can be constructed in terms of the trispectrum T and covariance matrix elements C :

$$N \equiv \sum_{LL'} N_{LL'} = f_{sky} \sum_{l_i m_i} \sum_{LM} \sum_{L'M'} (-1)^{M+M'} T_{l_3 l_4}^{l_1 l_2}(L) \begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & M \end{pmatrix} \begin{pmatrix} l_3 & l_4 & L \\ m_3 & m_4 & -M' \end{pmatrix} \\ \times T_{l_3 l_4}^{l_1 l_2}(L') \begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & M \end{pmatrix} \begin{pmatrix} l_3 & l_4 & L' \\ m_3 & m_4 & -M' \end{pmatrix} \{ C_{l_1 m_1, l_4 m_4}^{-1} C_{l_1 m_1, l_3 m_3}^{-1} C_{l_1 m_1, l_2 m_2}^{-1} C_{l_1 m_1, l_4 m_4}^{-1} + \text{cyclic permutation} \}. \quad (B5)$$

These results were used in construction of various estimators in the text of this paper. The estimators $E_l^{(3,1)}$ and $E^{(2,2)}$ that we construct therefore take the full trispectrum $T_{l_3 l_4}^{l_1 l_2}(L)$ into account and generalizes the estimators $K^{(3,1)}$ and $K^{(2,2)}$ where an approximate form was used.

APPENDIX C: $3j$ SYMBOLS

We list here various expressions related to $3j$ symbols (Edmonds 1968) that were used in the text:

$$\begin{pmatrix} l_2 & l_1 & l_3 \\ m_2 & m_1 & m_3 \end{pmatrix} = (-1)^{l_1+l_2+l_3} \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix}; \quad (C1)$$

$$\sum_{l_3 m_3} (2l_3 + 1) \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ m'_1 & m'_2 & m \end{pmatrix} = \delta_{m_1 m'_1} \delta_{m_2 m'_2}; \quad (C2)$$

$$\sum_{m_1 m_2} \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l'_3 \\ m_1 & m_2 & m'_3 \end{pmatrix} = \frac{\delta_{l_3 l'_3} \delta_{m_3 m'_3}}{2l_3 + 1}; \quad (C3)$$

$$(-1)^m \begin{pmatrix} l & l & l' \\ m & -m & 0 \end{pmatrix} = \frac{(-1)^l}{\sqrt{(2l+1)}} \delta_{l'0}. \quad (C4)$$

The Gaunt (or overlap) integral involving three spherical harmonics can be expressed in terms of $3j$ symbols as

$$\mathcal{G}_{m_1 m_2 m_3}^{l_1 l_2 l_3} \equiv \int d\hat{\Omega} Y_{l_1 m_1}(\hat{\Omega}) Y_{l_2 m_2}(\hat{\Omega}) Y_{l_3 m_3}(\hat{\Omega}) = \sqrt{\frac{(2l_1+1)(2l_2+1)(2l_3+1)}{4\pi}} \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix}. \quad (C5)$$

APPENDIX D: $6j$ SYMBOLS

The definition of $6j$ symbols in terms of the $3j$ symbols is as follows:

$$\begin{Bmatrix} l_1 & l_2 & L \\ l_3 & l_4 & L' \end{Bmatrix} = \sum_{m_i} \sum_{MM'} (-1)^{L+M+L'+M'} \begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & M \end{pmatrix} \begin{pmatrix} l_3 & l_4 & L \\ m_3 & m_4 & -M \end{pmatrix} \begin{pmatrix} l_1 & l_4 & L' \\ m_1 & m_4 & -M' \end{pmatrix} \begin{pmatrix} l_3 & l_2 & L \\ m_3 & m_4 & M' \end{pmatrix}. \quad (D1)$$

Various symmetries of $6j$ symbols can be found, for example, in Edmonds (1968).

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